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(54) Title: THREE-DIMENSIONAL MODEL OF A FC EPSILON RECEPTOR ALPHA CHAIN AND USES THEREOF

(57) Abstract

The present invention includes three-dimensional models of antibody receptor proteins, such as FccRI\alpha proteins, and methods to produce such models. The present invention also includes muteins having increased stability and/or antibody binding activity, as well as methods to produce such muteins, preferably using information derived from three-dimensional models of the present invention. Also included are nucleic acid sequences encoding muteins of the present invention and use of those sequences to produce such muteins. Also included is the use of the model to identify compounds that inhibit the binding of an antibody receptor protein to an antibody. The present invention also includes uses of such muteins and inhibitory compounds, for example, in methods to diagnose and protect animals from allergy and other abnormal immune responses.

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THREE-DIMENSIONAL MODEL OF A Fc EPSILON RECEPTOR ALPHA CHAIN AND USES THEREOF

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-FIELD OF THE INVENTION

The present invention relates to a crystal and a three-dimensional (3-D) model of a Fc epsilon receptor alpha chain as well as to the use of that model to produce muteins and inhibitors useful in the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

BACKGROUND OF THE INVENTION

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Antibody Fc-receptors (FcRs) play an important role in the immune response by coupling the specificity of secreted antibodies to a variety of cells of the immune system. A number of cell types, including macrophages, mast cells, eosinophils, and basophils, express membrane-bound FcRs at their surfaces. The binding of antibodies to FcRs provides antigen-specificity to these cells, which upon activation release further cell-specific mediators of the immune response, such as interleukins, initiators of inflammation, leukotrienes, prostaglandins, histamines, or cytotoxic proteins. The adoptive specificity of the FcRs allows a combinatorial approach to pathogen elimination, by coupling the diversity of antibody antigen-recognition sites to the variety of cell-types expressing these receptors.

FcR-initiated mechanisms are important in normal immunity to infectious disease as well as in allergies, antibody-mediated tumor recognition, autoimmune diseases, and other diseases in which immune responses are abnormal (i.e., not regulated). Recent experiments with transgenic mice have demonstrated that the FcRs control key steps in the immune response, including antibody-directed cellular cytotoxicity and inflammatory cascades associated with the formation of immune complexes; see, for example, Ravetch et al., 1998, *Annu Rev Immunolo 16*, 421-432. Receptors that bind IgG (FcgRI, FcgRII, and FcgRIII, known collectively as FcgRs) mediate a variety of inflammatory reactions, regulate B-cell activation, and also trigger hypersensitivity reactions. The high affinity Fc epsilon receptor (also known as the IgE

receptor or FceRI) is associated with the activation of mast cells and the triggering of allergic reactions and anaphylactic shock. Knockout mice for the FceRI alpha chain (FcεRIα) are unable to mount IgE-mediated anaphylaxis (see for example, Dombrowicz et al., 1993, Cell 75, 969-976), although FcgRs are still able to activate mast cells (see, for example, Dombrowicz et al., 1997, J. Clin. Invest. 99, 915-925; Oettgen et al., 1994, Nature 370, 367-370). FceRI has also been shown to trigger anti-parasitic reactions from platelets and eosinophils as well as deliver antigen into the MHC class II presentation pathway for the activation of T cells; see, for example, Gounni et al., 1994, Nature 367, 183-186; Joseph et al., 1997, Eur. J. Immunol. 27, 2212-2218; Maurer et al., 1998, J. Immunol. 161, 2731-2739. The b-subunit of FceRI has been associated with asthma in 10 genetic studies; see, for example, Hill et al., 1996, Hum. Mol. Genet. 5, 959-962; Hill et al., 1995, Bmj 311, 776-779; Kim et al., 1998, Curr. Opin. Pulm. Med. 4, 46-48; Mao et al., 1998, Clin. Genet. 53, 54-56; Shirakawa et al., 1994, Nat. Genet. 7, 125-129. A significant fraction of the population (~20%) may be affected by allergies, and this century has seen a substantial increase in asthma. Since IgE binding to FceRI is a requisite event in the reaction to different allergens, therapeutic strategies aimed at inhibiting FceRI could provide a useful treatment for these diseases. For example, monoclonal antibodies that target IgE and block receptor binding have shown therapeutic potential; see, for example, Heusser et al., 1997, Curr. Opin. Immunol. 9, 20 805-813.

FceRI is found as a tetrameric (abg₂) or trimeric (ag₂) membrane bound receptor on the surface of mast cells, basophils, eosinophils, langerhans cells and platelets. The alpha chain, also referred to as FceRIα, of FceRI binds IgE molecules with high affinity (K_D of about 10⁻⁹ to 10⁻¹⁰ moles/liter (M)), and can be secreted as a 172-amino acid soluble, IgE-binding fragment by the introduction of a stop codon before the single C-terminal transmembrane anchor; see, for example, Blank et al.,1991, E. J. Biol. Chem. 266, 2639-2646, which describes the secretion of a soluble IgE-binding fragment of 172 amino acids. The extracellular domains of the human FceRIα protein belong to the immunoglobulin (Ig) superfamily and contain seven N-linked glycosylation sites.

Glycosylation of FceRIα affects the secretion and stability of the receptor, but is not required for IgE-binding; see, for example, LaCroix et al., 1993, Mol. Immunol. 30,

321-330; Letourneur et al.,1995, J. Biol. Chem. 270, 8249-8256; Robertson, 1993, J. Biol. Chem. 268, 12736-12743; Scarselli et al., 1993, FEBS Lett 329, 223-226. The beta and gamma chains of FceRI are signal transduction modules.

Prior investigators have disclosed the nucleic acid sequence for human FceRIa: 5 see, for example, U.S. Patent No. 4,962,035, by Leder, issued October 9, 1990; U.S. Patent No. 5,639,660, by Kinet et al., issued June 17, 1997; Kochan et al., 1988, Nucleic Acids Res. 16, 3584; Shimizu et al., 1988, Proc. Natl. Acad. Sci. USA 85, 1907-1911; and Pang et al., 1993, J. Immunol. 151, 6166-6174. Nucleic acid sequences have also been reported for the human FceRI beta and gamma chains; see, respectively, Kuster et al., 1992, J. Biol. Chem. 267, 12782-12787; Kuster et al., 1990, J. Biol. Chem. 265, 10 6448-6452. Nucleic acid sequences have also been reported for nucleic acid molecules encoding canine FceRIa, murine FceRIa, rat FceRIa, feline FceRIa and equine FceRIa proteins; see, respectively, GenBank™ accession number D16413; Swiss-Prot accession number P20489 (represents encoded protein sequence); GenBank accession number J03606; PCT Publication No. WO 98/27208, by Frank et al., published June 25, 1998, 15 referred to herein as WO 98/27208; and PCT Publication No. WO 99/38974, by Weber et al., published August 5, 1999, referred to herein as WO 99/38974. In addition, methods to detect IgE antibodies using a FceRIa protein have been reported in PCT Publication No. WO 98/23964, by Frank et al., published June 4, 1998, referred to 20 herein as WO 98/23964; WO 98/27208, ibid.; PCT Publication No. WO 98/45707, by Frank et al., published October 15, 1998, referred to herein as WO 98/45707; and WO 99/38974, ibid.. WO 98/23964, WO 98/27208, WO 98/45707 and WO 99/38974.

There have been several reports of the use of mutagenesis and swapping techniques to attempt to identify amino acids of either FcεRIα or IgE involved in the binding of (i.e., interaction between) those respective proteins, reports attempting to model FceRIα proteins based on homology to other Ig-superfamily members, and reports that identify compounds that apparently inhibit such binding; see, for example, Cook et al., 1997, Biochemistry 36, 15579-15588; Hulett et al., 1994, J. Biol. Chem. 269, 15287-15293; Hulett et al., 1995, J. Biol. Chem 270, 21188-21194; Mallamaci et al., 1993, J. Biol. Chem. 268, 22076-22083; Robertson, 1993, ibid.; Scarselli et al., 1993, ibid. McDonnell et al., 1997, Biochem. Soc. Trans. 25, 387-392; McDonnell et al.,

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1996, Nat. Struc. Biol. 3, 419-426; PCT Publication No. WO 97/40033, by Cheng et al., published October 30, 1997; U.S. Patent No. 5,180,805, by Gould et al., issued January 19, 1993; U.S. Patent No. 5,693,758, by Gould et al., issued December 2, 1997; PCT Publication No. WO 96/01643, by Gould et al., published January 25, 1996; PCT Publication No. WO 95/14779, by Gould et al., published June 1, 1995. None of these references, however, describe isolated crystals of FcεRIα proteins or 3-D models derived from crystals.

Despite what is known about FcRs and their interaction with antibodies, there remains a need for FcRs with improved characteristics, such as enhanced affinity for antibodies, altered substrate specificity, increased stability, and increased solubility for use in diagnosis, treatment and prevention of allergy and other abnormal immune responses. Also needed for safe and efficacious compounds to prevent or treat allergy and to regulate other immune responses in an animal.

SUMMARY OF THE INVENTION

The present invention includes isolated crystals of the extracellular domains of antibody receptor proteins (FcRs), three-dimensional (3-D) models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as FcR muteins and other modified FcRs. Also included in the present invention are methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins. As such, the present invention includes FcRs with improved functions such as increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, including but not limited to reduced aggregation. Such proteins, also referred to as muteins, are useful to detect allergy and other intunue response abnormalities as well as to protect an animal from such abnormalities. The present invention also provides safe and efficacious inhibitory compounds to protect (e.g., prevent, treat, reduce the consequences of) an animal from allergy and to regulate other immune responses in an animal.

The present invention includes a 3-D model of an extracellular domain of a

human high affinity Fc epsilon receptor alpha chain (FceRIa) protein, wherein the model substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6,

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Table 7 or Table 8. The present invention also includes a 3-D model comprising a modification of a model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. Also included in the present invention are methods to produce such models.

The present invention also includes an isolated crystal of an extracellular domain of a FceRIa protein and methods to produce such a crystal.

The present invention also includes an isolated FceRIa protein consisting of SEQ ID NO:2 or of SEQ ID NO:4 except that the isoleucine at position 170 is replaced by a cysteine, as well as a protein that is structurally homologous to either such protein. Also included are nucleic acid molecules encoding such proteins, recombinant molecules and recombinant cells including such proteins, and methods to produce such proteins.

The present invention includes a method to identify a compound that inhibits the binding between an IgE antibody and a FcεRIα protein. The method includes the step of using a 3-D model of an extracellular domain of a human FcεRIα protein to identify the compound. Such a model substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. Also included in the present invention are inhibitory compounds identified using such a method. Also included are therapeutic compositions that include such inhibitory compounds and methods to use such therapeutic compositions to protect an animal from allergy or to regulate other immune responses (e.g., protect an animal from other abnormal immune responses).

The present invention also includes a mutein that binds to a Fc domain of an antibody. Such a mutein has an improved function compared to a protein that includes SEQ ID NO:2 or SEQ ID NO:4. Examples of such an improved function include increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, decreased aggregation, and increased solubility. Such a mutein is produced by a method that includes the following steps: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect an improved function of the protein; and (b) replacing the identified amino acid(s) to produce the mutein having such an improved function. The present invention also includes a mutein having an improved

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function compared to an unmodified FcεRIα protein, wherein the amino acid sequence of the mutein differs in at least one position from the amino acid sequence of the unmodified protein. Such a position(s) is in at least one of the following regions: a crystal contact cluster, a tryptophan-containing hydrophobic ridge, a FG loop in D2, a D1D2 interface, a cleft between D1 and D2, 2 domain 1, a domain 2, a hydrophobic core, a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, C'E loop of D2, a strand of D2, the amino terminal five residues of the protein, the carboxyl terminal five residues of the protein, and N-linked glycosylation sites.

Also included are muteins that are chemically modified FceRIa proteins. Also included are nucleic acid molecules that encode muteins of the present invention, recombinant molecules and recombinant cells including such nucleic acid molecules and methods to produce such muteins. Also included are diagnostic reagents and diagnostic kits including such muteins, therapeutic compositions including such muteins, and methods to detect or protect an animal from allergy or other abnormal immune responses.

The present invention also includes a method to improve a function of a FceRI α protein which includes the steps of: (a) analyzing a 3-D model of an extracellular domain of a human high affinity FceRI α protein substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8, to identify at least one amino acid of the protein which if replaced by a specified amino acid improves at least one of the functions of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having at least one of the improved functions.

BRIEF DESCRIPTION OF THE FIGURES

Fig. 1 depicts electron density maps and overall structure of a human FcεRIα model. (A) The 3.0 angstrom experimental electron density map, calculated using the MIRAS phases followed by density modification with the program DM is shown along with a refined model for human FcεRIα. The density is contoured at 1.4σ for residues 147-153. (B) Electron density for carbohydrate moieties linked to N42. The l2Fo-Fcl electron density map, contoured at 1σ, was calculated to 2.4 angstroms using combined MIRAS and model phases (prior to inclusion of carbohydrate in the model). Two N-acetylglucosamines and a mannose moiety were built into the density as shown.

- Fig. 2 depicts a ribbon diagram of a human FcεRIα model showing the positions of the disulfides and the FG loop in domain 2 (D2) that is implicated in receptor specificity. Domain 1 (D1) is shown to the right and D2 is shown to the left.
- Fig. 3 depicts a topology diagram of the two domains of a human FcεRIα model showing the hydrogen-bonding patterns of the beta sheet structure. The short stretch of parallel beta-sheet in D1 and D2 caused by the cross-over of the A strand is highlighted. Note that the FG strands of D2 are longer than those of D1, contributing to the prominence of the D2-FG loop.
- Fig. 4 demonstrates that a human FcεRIα model has a novel tertiary arrangement of tandem Ig domains.
 - Fig. 5 depicts sequence alignments of human FcRs. The secondary structure of the two domains is indicated with labeled bars above those residues which form beta-sheet in FcɛRI. Below the sequences, carbohydrate attachment sites found in seventeen different FcR sequences are indicated with a (+). This analysis is based on the seven human receptors shown and the non-human receptors listed in Table 4.
 - Fig. 6 depicts the four surface-exposed tryptophans at the top of the D2 domain of a human FcεRIα model that are implicated in IgE binding.

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- Fig. 7 depicts residues in the D2 FG loop and D1 E strand of a human FcεRIα model that are highly variable in human FcR sequences. The residues in the D2-FG loop have been directly implicated in IgE binding. The residues in the D1 E strand and the D1 A'B loop are located near the top of the D2 domain and could form part of an extended IgE-binding surface between the two domains.
- Fig. 8 depicts a juxtaposition of a human FcεRIα model with a model for the intact IgE antibody structure. The insertion of the Cε2 domains in the IgE molecule are indicated by dotted lines. The FcεRIα protein is shown relative to the mast cell membrane near the top of the Cε3 domains that bind to the receptor.

DETAILED DESCRIPTION OF THE INVENTION

The present invention includes isolated crystals of the extracellular domains of FcRs, 3-D models of such crystals and modifications of such models. The present invention also includes compounds that inhibit the ability of FcRs to bind to antibodies as well as muteins and other modified FcRs. Also included in the present invention are

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methods to produce and use such crystals, models, inhibitory compounds, muteins, and other modified proteins.

The present invention includes an isolated crystal of an extracellular domain of a high affinity Fc epsilon receptor alpha chain (FceRIa), a 3-D model of such a crystal and a modification of such a model. As used herein, the term "a" entity or "an" entity refers to one or more of that entity; for example, a crystal or a model refers to one or more crystals or models, respectively. As such, the terms "a" (or "an"), "one or more" and "at least one" can be used interchangeably herein. It is also to be noted that the terms "comprising", "including", and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of' refers to one or more of the compounds in the list that follows, including mixtures, or combinations, of two or more of the compounds.

As used herein, an extracellular domain of a Fc ϵ RI α protein is the portion of the FceRI alpha chain that is exposed to the environment outside the cell and that binds to the Fc domain of an IgE antibody. Such an extracellular domain can be (a) a complete extracellular domain which is a domain that extends from the first amino acid of a mature FceRI alpha chain through the last amino acid prior to the start of the transmembrane region or a domain that is functionally equivalent, in that such a domain includes a D1 and D2 domain, displays a similar affinity for the IgE antibody to which such an FcεRIα protein naturally binds, and produces crystals having sufficient quality to enable structure determination, or (b) a fragment of any of the extracellular domains of (a), wherein the fragment retains its ability to bind to the Fc domain of an antibody. As used herein, the terms binding to an antibody and binding to the Fc domain (i.e., constant region) of an antibody can be used interchangeably since it is recognized that a FcR binds to the Fc domain of an antibody. A FcR (i.e., a protein that can bind to an antibody), such as a FceRIa protein, can be a full-length FcR (e.g., a full-length FceRI alpha chain), or any fragment thereof, wherein the fragment binds to an antibody. Similarly an antibody, or an Fc domain thereof, can be a full-length antibody, or fulllength Fc domain thereof, or any fragment thereof that binds to a FcR. Preferably a FcR binds to an antibody with an affinity (K_A) of at least about 10⁸ liters/mole (M⁻¹), more 30 preferably of at least about 10° M⁻¹, and even more preferably of at least about 10¹⁰ M⁻¹.

The present invention is surprising in several aspects. For example, this is the first report of an isolated crystal of an extracellular domain of a FceRIa protein, and in particular of an isolated crystal of sufficient quality that a crystal structure, i.e., a 3-D model, could be derived therefrom. The inventors believe that this protein also represents the most highly glycosylated protein for which a crystal and a 3-D model have 5 been reported to date. Not only does glycosylation interfere with protein crystal formation but it also is difficult to consistently produce recombinant proteins having a uniform glycosylation pattern. Generation of such a crystal was very difficult and nonobvious and has been attempted by others without success. The inventors tried many approaches before discovering that a preferred FceRIa protein from which to make a useful crystal is a FceRIa protein that consists of amino acids 1 through 176 of the mature human FceRIa protein. This protein is denoted herein as PhFceRIa₁₋₁₇₆, or the hFcεRIα₁₋₁₇₆ protein, and has an amino acid sequence denoted herein as SEQ ID NO:2. An example of a nucleotide acid molecule encoding PhFceRIa₁₋₁₇₆ is referred to herein as nhFceRIa₁₋₅₂₈, the nucleic acid sequence of which is denoted herein as SEQ ID NO:1. It was also discovered that better crystals are generated when PhFcεRIα₁₋₁₇₆ is produced in insect cells, using a method such as that described in the Examples. Determination of the crystal structure of PhFceRIa₁₋₁₇₆ produced in Trichoplusia ni (Hi-5) cells resulted in a 3-D model that substantially represents the atomic coordinates specified in Table 1, referred to herein as form M1. Amino acids are represented herein by their standard 20 three or one letter codes; see, for example, Sambrook et al., Molecular Cloning: A . Laboratory Manual, Cold Spring Harbor Labs Press, 1989. Prior to obtaining a crystal of sufficient quality to solve its crystal structure using insect-cell produced PhFceRI α_1 . 176, a number of other proteins were tried, including a FceRIa protein spanning from amino acid 1 through 171 of SEQ ID NO:2 produced in Pichia pastoris, and FceRIa 25 proteins spanning from amino acid 1 through 172 of SEQ ID NO:2 produced in Chinese hamster ovary cells, Trichoplusia ni cells, and Spodoptera frugiperda cells without success. Without being bound by theory, it is believed that PhFceRIa₁₋₁₇₆ was a better candidate because it apparently represents a complete extracellular domain. Based on the 3-D model of PhFceRI α_{1-176} , the inventors believe, without being bound by theory, that the amino acid at position 172 is important in the structure determination and that,

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in order to form a crystal of sufficient quality to determine the first 3-D model of a FceRIa protein, at least one additional amino acid was required carboxyl-terminal to that at position 172; the inventors further believe that an optimal protein would span from the amino acid at position 3 through the amino acid at position 174 of SEQ ID NO:2. It

should be noted, however, that having solved the crystal structure of a first FceRI\u03e9 protein enables the solving of crystal structures of additional FceRI\u03e9 proteins as well as of additional FcRs in general. For example, the crystal structures of two additional crystals cited in the Examples can be solved using a combination of X-ray diffraction data of the crystals per se and information derived from the 3-D model of PhFceRI\u03e9₁₋₁₇₆.

The examples also describe the solution of an additional four crystal structures using such information, namely the examples present 3-D models of: (a) a human FceRI α protein spanning amino acids 1-172 of SEQ ID NO:2 (i.e., PhFceRI α_{1-172} , the amino acid sequence of which is represented herein as SEQ ID NO:4) expressed in lec1 Chinese hamster ovary (CHO) cells, the structural form being referred to herein as Form T1; (b) a second structural form of PhFceRI α_{1-172} produced in lec1 CHO cells, referred to herein as Form T2; (c) a second structural form of a PhFceRI α_{1-176} protein expressed in *T. ni* (Hi5) cells, referred to herein as Form M2; and (d) a PhFceRI α_{1-172} protein in which the isoleucine at position 170 of SED ID NO:4 is replaced with a cysteine, expressed in Sf9 insect cells, a structural form referred to herein as H1. The atomic coordinates of the crystal structural forms T1, T2, M2 and H1 are presented, respectively, in Tables 5, 6, 7,

The 3-D model of the hFceRI α_{1-176} protein form M1 is also very surprising in view of the knowledge of the structure of proteins containing immunoglobulin domains, herein also referred to as Ig domains. The most striking differences, which are described in greater detail below, include, but are not limited to: domain 1 (D1) and domain 2 (D2) of the model of PhFceRI α_{1-176} are much smaller than known Ig domains; the packing and orientation of D1 and D2 of the hFceRI α_{1-176} protein are significantly different from known Ig domain-containing proteins in that, for example, the bend angle between D1 and D2 of the PhFceRI α_{1-176} structure is much more acute than for other proteins, the relative rotational orientation of the two domains is much different, D1 and D2 of PhFceRI α_{1-176} form an unusual interface and cleft, D1 and D2 of PhFceRI α_{1-176} are

antiparallel, the presence of a hydrophobic surface on the two faces of the model of PhFcεRIα₁₋₁₇₆ which appear to be nearby or directly involved in binding to IgE antibodies; the FG loop of D2 of PhFc ϵ RI α_{1-176} , also apparently involved in binding to IgE antibodies, projects much more significantly above the D2 domain than is seen for known D2-containing proteins; and the interruption in structure between strands A and A' in D1 which apparently leads to interaction between the two domains. It is to be noted that although most known Ig domain pairs which are parallel, some Ig domains are antiparallel (e.g., hemolin) but the domain:domain orientation and specifics of packing of those domains are very different from the orientation and packing of PhFceRI α_{1-176} . It is also surprising that the model of the hFc ϵ RI α_{1-176} protein predicts that an IgE antibody interacts with D1 as well as D2 in view of the mutagenesis analysis studies conducted to date all of which have only identified mutations in D2 that lead to decreased, or increased, binding between a FceRIa protein and an IgE antibody. As such, a model of the present invention is necessary for proper interpretation and refinement of mutagenesis and region swapping studies that have been reported. Such a model for the first time permits the differentiation between amino acids directly or indirectly influencing binding of IgE to FceRIa and demonstrates where amino acids and amino acid segments identified in mutagenesis and swapping studies are positioned on the protein. It is to be noted that the 3-D models of FceRIa crystal structure forms T1, T2, M2 and H1 are quite similar to that of form M1, with the following differences. The principal differences in the structures from the various crystal forms occur in the BC loop in domain 1 (the "30 loop"), the C' strand in domain 2 (the "130 region") and the carbohydrate sites. There are also smaller differences in the termini of the structures and the FG loop in domain 1 (the "72 loop"). These differences are described in more detail 25

One embodiment of the present invention is an isolated crystal of an extracellular domain of a FceRI\alpha protein. As used herein, an isolated crystal is a crystal of a protein that has been produced in a laboratory; that is, an isolated crystal is produced by an individual and is not an object found in situ in nature. It is appreciated by those skilled in the art that there are a variety of techniques to produce crystals including, but not limited to, vapor diffusion using a hanging or sitting drop methodology, vapor diffusion

under oil, and batch methods; see, for example, Ducruix et al., eds., 1991, Crystallization of nucleic acids and proteins; A practical approach, Oxford University Press, and Wyckoff et al., eds., 1985, Methods in Enzymology 11, 49-185. It is also to be appreciated that crystallization conditions can be adjusted depending on a protein's inherent characteristics as well as on a protein's concentration in a solution and that a variety of precipitants can be added to a protein solution in order to effect crystallization; such precipitants are known to those skilled in the art. In a preferred embodiment, a crystal of a FceRIa protein is produced in a solution by adding a precipitant such as polyethylene glycol (PEG) or PEG monomethylether. In a particularly preferred embodiment, the precipitant PEG is added to .. solution to achieve a final concentration of from about 10 percent (%) to about 40%, preferably from about 12% to about 32% PEG per volume solution. It is also to be noted that a $FceRI\alpha$ protein used to produce a crystal can be produced by a variety of methods, including purification of a native protein, chemical synthesis of a protein, or recombinant production of a protein. Although a number of cell types can be used to recombinantly produce such a protein, insect cells, such as, but not limited to Trichoplusia ni and Spodoptera frugiperda, are preferred, with Trichoplusia ni cells being more preferred. Also preferred are Chinese hamster ovary cells. Additional methods to produce proteins are disclosed below.

Isolated crystals of the present invention can include heavy atom derivatives,
such as, but not limited to, gold, platinum, mercury, selenium, and lead. Such heavy atoms can be introduced randomly or introduced in a manner based on knowledge of 3-D models of the present invention. Additional crystals of the present invention are not derivatized. In one embodiment, an isolated crystal of the present invention is a cocrystal of a FceRIα protein bound to a Fc domain of an IgE antibody. In another embodiment, an isolated crystal of the present invention is a co-crystal of a FceRIα protein and a compound that inhibits the binding of a FceRIα protein to a Fc domain of an IgE antibody. Additional crystals of the present invention include crystals produced from proteins that are muteins of the present invention or other proteins that are represented by a 3-D model of the present invention.

An isolated crystal of the present invention can be the crystal of any suitable extracellular domain of a FceRI\alpha protein. Suitable FceRI\alpha proteins include mammalian

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FcεRIα proteins, with human, canine, feline, equine, rat and murine FcεRIα proteins being preferred, and human FceRIa proteins being even more preferred. A preferred crystal of the present invention diffracts X-rays to a resolution of about 4.0 angstroms or higher (i.e., lower number meaning higher resolution), with resolutions of about 3.5 angstroms or higher, about 3 angstroms or higher, about 2.5 angstroms or higher, about 2 angstroms or higher, about 1.5 angstroms or higher, and about 1 angstrom or higher being increasingly more preferred. It is appreciated, however, that additional crystals of lower resolutions can have utility in discerning overall topology of the structures, e.g., location of a binding site or where a molecule binds to a receptor. A particularly preferred isolated crystal of the present invention has the amino acid 10 sequence SEQ ID NO:2, amino acid sequence SEQ ID NO:4, or a sequence essentially equivalent that represents an extracellular domain of another mammalian $FceRI\alpha$ protein. SEQ ID NO:4 is the amino acid sequence of a protein consisting of the first 172 residues of a mature human FcεRIα protein denoted herein as PhFcεRIα₁₋₁₇₂; i.e., SEQ ID NO:4 spans from amino acid residue 1 through amino acid residue 172 of SEQ ID 15 NO:2. An example of a nucleotide acid molecule encoding PhFceRI α_{1-172} is referred to herein as nhFceRIa₁₋₅₁₆, the nucleic acid sequence of which is denoted herein as SEQ ID NO:3. Preferred are crystals that belong to monoclinic space group C2 or monoclinic space group P6122. Particularly preferred crystals include: a crystal of PhFc ϵ RI α_{1-176} that belongs to monoclinic space group C2, has cell dimensions of 88.6 angstroms x 69.6 angstroms x 49.3 angstroms, alpha=gamma=90.0 degrees, beta=116.69 degrees, and diffracts X-rays to a resolution of about 2.4 angstroms (form M1); a crystal of PhFceRI α_{1-176} that belongs to monoclinic space group C2, has cell dimensions of 136.02 angstroms x 75.01 angstroms x 79.28 angstroms, alpha=gamma=90 degrees, beta=117.8 degrees, and diffracts X-rays to a resolution of about 3.0 angstroms; and a crystal of 25 PhFceRIα₁₋₁₇₂ that belongs to monoclinic space group P6122, has cell dimensions of 58 angstroms x 58 angstroms x 226 angstroms, alpha=beta=90 degrees, gamma=120 degrees, and diffracts X-rays to a resolution of about 3.2 angstroms. Also preferred crystals include: a crystal of PhFceRIa₁₋₁₇₂ that belongs to tetragonal space group P4₃, has cell dimensions of 145.08 angstroms x 145.08 angstroms x 62.74 angstroms, 30 alpha=beta=gamma=90.0 degrees, and diffracts X-rays to a resolution of about 3.1

angstroms (form T1); a crystal of PhFcεRIα₁₋₁₇₂ that belongs to tetragonal space group P4₃, has cell dimensions of 150.50 angstroms x 150.50 angstroms x 74.18 angstroms, alpha=beta=gamma=90.0 degrees, and diffracts X-rays to a resolution of about 3.8 angstroms (form T2); a crystal of PhFcεRIα₁₋₁₇₆ that belongs to monoclinic space group C2, has cell dimensions of 136.90 angstroms x 73.79 angstroms x 79.40 angstroms, c1 alpha=gamma=90.0 degrees, beta=117.74 degrees, and diffracts X-rays to a resolution of about 3.2 angstroms (form M2); and a crystal of PhFcεRIα₁₋₁₇₂ that belongs to hexagonal space group P6₁22, has cell dimensions of 58.62 angstroms x 58.62 angstroms x 229.19 angstroms, alpha=gamma=90.0 degrees, beta=120 degrees, and diffracts X-rays to a resolution of about 3.2 angstroms (form H1)

The present invention includes a 3-D model of an extracellular domain of a FcεRIα protein that substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. The present invention also includes 3-D models that comprise modifications of the model substantially represented by the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8. Each such modification represents a protein that binds to a Fc domain of an antibody. A 3-D model of an extracellular domain of a FceRIa protein is a representation, or image, that predicts the actual structure of the corresponding protein. As such, a 3-D model is a tool that can be used to probe the relationship between the protein's structure and function at the atomic level and to design muteins (i.e., genetically and/or chemically altered FcRs) having an improved function, such as, but not limited to: increased (i.e., enhanced) 20 stability; increased antibody binding activity, for example, by, increasing the affinity for an antibody by, for example, increasing the association rate and/or decreasing the dissociation rate between a FcR and an antibody or by altering substrate specificity (e.g., enhancing the ability of a FcR of a certain species and class to bind to antibody from another species and/or another antibody class); and/or increased solubility (e.g., reduced 25 aggregation). It is well known to those skilled in the art, however, that a 3-D model of a protein derived by analysis of protein crystals is not identical to the inherent structure of the protein. See, for example, Branden et al., Introduction to Protein Structure, Garland Publishing Inc., New York and London, 1991, especially on page 277, which states "not surprisingly the model never corresponds precisely to the actual crystal." Furthermore, 30

the model can be subjected to further refinements to more closely correspond to the actual structure of a FcR. Such a refined model, which is an example of a modification of the present invention, is a better predictor of the actual structure and mechanism of action of the protein that the model represents. A refinement of a 3-D model of the present invention refers to an improved model of a FccRI\u03c3 protein that can be obtained in a variety of ways known to those skilled in the art. Refinements can include models determined to more preferred degrees of resolution, preferably to about 3.5 angstroms, more preferably to about 3 angstroms, more preferably to about 2 angstroms, more preferably to about 1 angstroms, more preferably to about 1 angstrom. Preferred refinements are obtained using the 3-D model as a basis for such improvements.

One embodiment of the present invention is a 3-D model of an extracellular domain of a FceRIa protein that substantially represents the atomic coordinates specified (i.e., listed) in Table 1.

Table 1. Atomic coordinates of PhFceRIa₁₋₁₇₆, Form M1

ATOM	ATOM TYPE	RESIDUE	#	_x_	<u>Y</u>	_ <u>z</u>	<u>occ</u>	<u>B</u>
NUMBER 1 5 2	CB CG	LYS LYS	4	23.345 23.455 23.900	19.877 20.034 21.4 44	27.253 25.744 25.387	1.00 1.00 1.00	114.16 114.16 114.16 114.16
3 4	CD	LYS LYS LYS	4 4 4	24.017 24.406	21.633 23.028	23.885 23.539 27.171	1.00 1.00 1.00	114,16 98.73
5 6 10 7	NZ C O	LYS LYS	4	23.899 24.999 22.817	17.439 17.777 18.457	26.726 29.211	1.00 1.00	98.73 98.73 98.73
8 9	N CA	LYS LYS PRO	4 4 5	22.920 23.522	18.482 16.148	27.721 27.224 27.963	1.00 1.00 1.00	89.31 81.52
10 11 15 12	N CD CA	PRO PRO	5 5 5	22.385 24.397 23.912	15.565 15.093 13.858	26.708 27.454	1.00 1.00	89.31 81.52 81.52
15 12 13 14	CB CG	PRO PRO PRO	5 5 5	22.445 24.212	14.102 14.980	27.562 25.190 24.581	1.00 1.00 1.00	89.31 89.31
15 16 20 17	C O N	PRO LYS	5 5 6	23.503 24.844 24.719	15.784 13.992 13.835	24.575 23.137	1.00 1.00	79.33 79.33 122.37
18 19	CA CB	LYS LYS LYS	6 6 6	25.816 25.411	14.639 15.180	22.433 21.073 20.643	1.00 1.00 1.00	122.37 122.37
20 21 25 22	CG CD CE	LYS LYS	6 6 6	26.324 25.774 26.602	16.320 17.040 18.225	19.421 19.060	1.00 1.00 1.00	122.37 122.37 79.33
23 24	NZ C O	LYS LYS LYS	6 6	24.794 25.644	12.368 11.622 11.948	22.740 23.231 21.866	1.00 1.00	79.33 65.03
25 26 30 27	N CA	VAL VAL	7 7 7	23.884 23.879 22.479	10.567 10.128	21.409 20.951 20.408	1.00	65.03 74.25 74.25
28 29 30	CB CG CG	1 VAL	7 7	22.530 21.515 24.846	8.711 10.205 10.463	22.113 20.24	1.00	74.25 65.03 65.03
31 35 32	C	VAL VAL SER	7 7 8	24.829 25.713	11.290 9.462	19.328 20.299 19.23	9 1.00	46.54 46.54
33 34 35	N CA CE	SER SER	8	26.686 28.123 28.482	9.513	19.74 20.83	9 1.00 6 1.00	64.02 64.02
36 40 37	0(C 0	SER	8	26.517 26.109	7.815 6.955	18.78 19.56 17.51	7 1.00	46.54 55.36
38 39 40	N C	A LEU	, 9	26.674	6.227 6.283	16.94 15.67	1.00 79 1.00	0 45.99
41 45 42 43	C	B LEU G LEU D1 LEU	j :	24.62	6 7.256 3 6.849	15.55 14.3 16.7	38 1.0 61 1.0	0 45.99 0 45.99
44 45	C	D2 LEI	زُ	9 23.78 9 27.98 9 28.89	3 5.585 4 6.250	16.5 16.0 16.7	91 1.0	00 55.36 00 52.82
46 50 47 48	1	N AS	N N	10 28.06 10 29.24	14 3.556 74 3.353	16.3 17.5	1.0 10 1.0	00 52.82 00 77.87
49 50		CB AS CG AS OD1 AS	in	10 31.30 10 32.00	56 2.495 32 2.717	17.1 16.1 18.1	155 1.0 004 1.0	00 77.87 00 77.87
51 55 52 53		ND2 AS	SN	10 31.6 10 28.8 10 28.3	16 2.215 20 1.361	15. 16.	753 1. 492 1.	00 52.82 00 52.82 00 54.26
54 55 56		N PI	RO RO	11 28.9 11 28.7	966 2.024 755 0.707	13. 13.	793 1. 454 1.	.00 46.78 .00 54.26
60 57 58		CA P	RO RO	11 29.5 11 29.5	,00	9 12	.155 1	.00 46.78

	59 60 61	CG C	PRO PRO	11 11	29.707 28.692 27.541	0.774 4.268 4.332 5.303	12.631 13.348 13.775 12.742	1.00 1.00 1.00	46.78 54.26 54.26 56.88
5	62 63 64 65	N CD CA CB	PRO PRO PRO PRO	12 12 12 12	29.286 30.615 28.751 29.888 31.093	5.189 6.646 7.348 6.592	12.120 12.514 11.788 12.191	1.00 1.00 1.00 1.00	56.23 56.88 56.23 56.23
	66 67	C C	PRO PRO	12 12	27.458 26.680	6.798 7.710	11.736 12.003	1.00 1.00	56.88 56.88
10	68	0 N	PRO TRP	12 13	27.255	5.930 5.991	10.751 9.881	1.00 1.00	54.29 54.29
	69 70	CA CB	TRP TRP	13 13	26.079 26.203	4.929	8.794 8.423	1.00 1.00	47.07 47.07
	71 72	CG	TRP	13 13	27.629 28.502	4.697 5.622	7.767	1.00	47.07 47.07
15	73	CD2 CE2	TRP TRP	13	29.762	4.998	7.659 7.266	1.00 1.00	47.07 47.07
	74 75	CE3	TRP	13	28.341 28.372	6.919 3.584	8.676	1.00	47.07
	76	CD1 NE1	TRP TRP	13 13	29.655	3.756	8.218 7.064	1.00 1.00	47.07 47.07
20	77 78	CZ2	TRP	13	30.853 29.419	5.62 - 7.536	6.679	1.00	47.07
20	79	CZ3	TRP TRP	13 13	30.664	6.890	6.582	1.00 1.00	47.07 54.29
	80	CH2 C	TRP	13	24.753	5.836 4.312	10.602 11.389	1.00	54.29
	81 82	0	TRP	13	24.571 23.838	6.759	10.323	1.00	44.90
25	83	N CA	ASN ASN	14 14	22.513	6.758	10.925 11.291	1.00 1.00	44.90 62.66
	84 85	CB	ASN	14	22.099	8.179 8.992	10.083	1.00	62.66
	86	CG	ASN ASN	14	21.713 22.501	9.154	9.152	1.00 1.00	62.66 62.66
20	87	OD1 ND2	ASN	14	20.489	9.505 6.158	10.085 9. 93 5	1.00	44.90
30	88 89	С	ASN	14 14	21.504 20.302	6.059	10.229	1.00	44.90 43.26
	90	0 N	ASN ARG	15	22.006	5.777	8.759 7.735		43.26 43.26
	91 92	CA	ARG	15	21.189	5.130 5.926	6.426	1.00	51.24
35		CB	ARG	15 15	21.196 21.031	7.419	6.623	1.00	51.24 51.24
	94	CG CD	ARG ARG	15	21.112	8.161	5.311 4.637		51.24
	95 96	NE	ARG	15	19.813 19.648	8.119 7.770	3.375	1.00	51.24
	97	CZ NH1	ARG ARG	15 15	20.693	7.441	2.652 2.849		51.24 51.24
4	0 98 99	NH2	ARG	15	18.442	7.743 3.799	7.54	5 1.00	43.26
	100	С	ARG	15 15	21.902 23.017	3.759	7.03	1 1.00	43.26 47.47
	101	0 N	ARG ILE	10	21.258	2.719	7.98 7.89		47.47
4	102 5 103	CA	ILE	10		1.386 0.864	9.30	8 1.00	38.74
	104	CB	ILE ILE	1.		1.866	10.02		38.74 38.74
	105 106	CG2 CG1		1	6 20.944	0.673 0.154	10.13 11.56	8 1.00	38.74
	107	CD1	ILE		6 21.166 6 20.912	0.357	7.2	57 1.00	47.47 47.47
:	50 108	C	ILE ILE	1	6 19.711	0.579	7.1° 6.9		45.27
	109 110	Ň	PHE		7 21.480 17 20.721		6.3	09 1.00	45.27
	111	CA	PHE		17 20.721 17 21.636	-2.758	5.4		33.04 33.04
	112 55 113	CB CG		•	17 21.911		4.1 3.5		33.04
	114	CD	1 PHE		17 23.185 17 20.864	4	3.3	22 1.00	
	115	CD: CE	2 PHE 1 PHE		17 23.43	2 -1.782	2.3	307 1.00 36 1.00	
	116 117	CE	2 PHE		17 21.10 17 22.38		1.5	523 1. 0 0	33.04
	60 118	CZ	PHE		17 22.38 17 20.02	6 -2.748	7.3	334 1.00	
	119 120	CO	PHE		17 20.54			433 1.00 959 1.00	48.86
	121	N	LYS		18 18.84 18 18.07			806 1.00	48.86
	122	CA	LYS		,=				

						-4.630			55.91
12	23		LYS		16.848 16.039	-5.694	7.731	1.00	55.91 ·
12	24	-	LYS LYS		14.629	-5.696	• • • • -		55.91 55.91
	25	CD	LYS	18	13.744	-6.718 -0.75	7.865 7.298	1.00	55.91
	26 · 27	NZ	LYS	18	13.936	-8.075 -5.2 99	8.149	1.00	48.86
	27 28	С	LYS	18	19.003 19.635	-5.875	7.267	1.00	48.86
1	29	0	LYS GLY	18 19	19.106	-5.627	9.429	1.00 1.00	53.46 53.46
	30	N CA	GLY	19	19.993	-6.705	9.832 10.311	1.00	53.46
10 1	31 32	C	GLY	19	21.381	-6.284 -7.117	10.837	1.00	53.46
10 1	33	Ŏ	GLY	19	22.111 21.758	-5.016	10.134	1.00	46.04 46.04
1	134	N	GLU GLU	20 20	23.073	-4.533	10.576	1.00 1.00	45.53
	135	CA CB	GLU	20	23.553	-3.372 - 671	9.700 8.197	1.00	45.53
	136 137	CG	GLU	20	23.544 24.253	-3.671 -2.611	7.347	1.00	45.53
	138	CD	GLU	20 20	24.253 24.049	-1.393	7.587	1.00	45.53 45.53
	139	OE1	GLU GLU	20	25.008	-3.004	6.423 12.039	1.00 1.00	46.04
	140	OE2 C	GLU	20	23.046	-4.083 -3.958	12.039	1.00	46.04
20	141 142	J	GLU	20	21.980 24.223	-3.936 -3.845	12.607	1.00	50.99
20	143	N	ASN	21 21	24.223	-3.422	13.994	1.00	50.99 67.08
	144	CA	ASN ASN	21	25.255	-4.321	14.790 14.825	1.00 1.00	67.08
	145	CB CG	ASN	21	24.817	-5.776 -6.077	15.049	1.00	67.08
25	146 147	OD1	ASN	21	23.634 25.782	-6.675	14.619	1.00	67.08
25	148	ND2	ASN	21 21	24.765	-1.985	14.118	1.00	50.99 50.99
	149	C	ASN ASN	21	25.533	-1.493	13.290 15.164	1.00 1.00	48.02
	150 151	N	VAL	22	24.291	-1.317 0.058	15.453	1.00	48.02
30	152	CA	VAL	22	24.674 23.752	1.086	14.742	1.00	39.09 39.09
50	153	CB	VAL VAL	22 22	22.313	0.924	15.215	1.00 1.00	39.09
	154	CG1 CG2	VAL	22	24.243	2.499	15.023 16.964	1.00	48.02
	155 156	C	VAL	22	24.552 23.568	0.241 -0.203	17.577	1.00	48.02
35	157	0	VAL	22 23	25.558	0.870	17.570	1.00	52.73 52.73
	158	N	THR THR	23	25.530	1.102	19.013 19.686		65.60
	159 160	CA CB	THR	23	26.848	0.666 -0.754	19.570	1.00	65.60
	161	OG1	THR	23	26.999 26.849	1.059	21.162	1.00	65.60
40	162	CG2	THR THR	23 23		2.577	19.294		52.73 52.73
	163	C	THR	23	25.946	3.422	18.673 20.214		47.77
	164 165	N	LEU	24		2.883 4.267	20.576	1.00	47.77
	166	CA	LEU	24 24		4.561	20.54		58.94 58.94
45	167	CB	LEU LEU	24	21.813	4.200	19.30 19.40		58.94
	168	CG CD1	LEU	24	20.429	4.824 4.704	18.06		58.94
	169 170	CD2	LEU	24			21.98	0 1.00	47.77
	171	C	LEU	2. 2.		3.858	22.95		47.77 57.92
50		0 N	THR	2	5 25.5 6 3		22.08 23.37		57.92
	173 174	CA	THR	2			23.31	1.00	61.52
	175	CB	ים אב ים הל		5 27.700 5 28.091	4 440	22.99	95 1.00	61.52 61.52
_	176	OG1			5 28.29	2 6.164	24.60 23.8		57.92
5:	5 177 178	CG2 C	THR	2	25 25.73		23.0 23.0		57.92
	179	ŏ	THR		25.73		25.1	01 1.00	87.83
	180	N	CYS		26 25.39 26 24.99		25.6		
	181	CA	CYS CYS		26 26.31	9 9.363	26.0 26.2	31 1.00 56 1.00	
6	0 182 183	C	CYS	:	26 27.33		26.2 26.9		68.33
	184	CB	CYS	1	26 24.14 26 23.11		27.5	559 1.00	
	185	SG			26 23.11 27 26.31		26.0	067 1.00	98.51
	186	N	ASN						

		CA	ASN	27 .	27.538	11.474	26.307	1.00 1.00	98.51 123.41
	187	CB	ASN	27	27.183	12.865	26.803		123.41
	188	CG .	ASN	27	27.922	13.945	26.038	1.00	123.41
	189	OD1	ASN	27	29.067	13.760	25.618	1.00	123.41
	190	ND2	ASN	27	27.268	15.085	25.851 27.174	1.00	98.51
	191 192	C	ASN	27	28.671	10.911	27.174	1.00	98.51
	192	Ö	ASN	27	28.481	9.968	27. 9 57 27.053	1.00	112.08
	193	Ň	GLY	28	29.849	11.531	27.774	1.00	112.08
	195	CA	GLY	28	31.050	11.111	29.235	1.00	112.08
10	196	C	GLY	28	31.283	11.487	29.874	1.00	112.08
10	197	Ö	GLY	28	32.175	10.929 12.430	29.772	1.00	117.67
	198	N	ASN	29	30.513	12.430	31.175	1.00	117.67
	199	CA	ASN	29	30.674	14.176	31.464	1.00	132.23
	200	СВ	ASN	29	30.018	15.301	30.619	1.00	132.23
15	201	CG	ASN	29	30.579	15.505	30.559	1.00	132.23
	202	OD1	ASN	29	31.792 29.693	16.049	29.971	1.00	132.23
	203	ND2	ASN	29	30.009	11.779	32.077	1.00	117.67
	204	С	ASN	29	30.259	11.737	33.277	1.00	117.67
	205	0	ASN	29	29.158	10.943	31.489	1.00	110.72
20	206	N	ASN	30	28.423	9.921	32.235	1.00	110.72
	207	CA	ASN	30	27.236	9.430	31.395	1.00	135.09
	208	СВ	ASN	30	26.331	8.468	32.153	1.00	135.09
	209	CG	ASN	30 30	26.684	7.989	33.231	1.00	135.09
	210	OD1	ASN	30	25.163	8.183	31.590	1.00	135.09
25	211	ND2	ASN	30	29.267	8.721	32.680	1.00	110.72
	212	C	ASN ASN	30	29.834	8.000	31.853	1.00	110.72
	213	0	PHE	31	29.338	8.509	33.995	1.00	129.04 129.04
	214	N	PHE	31	30.095	7.397	34.559	1.00	95.73
	215	CA CB	PHE	31	31.178	7.900	35.519	1.00 1.00	95.73
30	216	CG	PHE	31	32.321	8.589	34.837	1.00	95.73
	217	CD1	PHE	31	32.106	9.716	34.059	1.00	95.73
	218	CD2	PHE	31	33.619	8.127	34. 993 33.440	1.00	95.73
	219 220	CE1	PHE	31	33.166	10.380	34.378	1.00	95.73
35	220 221	CE2	PHE	31	34.687	8.784	33.603	1.00	95.73
33	222	CZ	PHE	31	34.458	9.915	35.308	1.00	129.04
	223	Č	PHE	31	29.181	6.440	35.908	1.00	129.04
	224	Ö	PHE	31	28.188	6.850 5.1 6 0	35.260	1.00	141.76
	225	N	PHE	32	29.531	4.109	35.937	1.00	141.76
40		CA	PHE	32	28.775	2.765	35.876	1.00	141.76
	227	CB	PHE	32	29.529 30.787	2.788	35.031	1.00	141.76
	228	CG	PHE	32	31.814	3.706	35.280	1.00	141.76
	229	CD1	PHE	32	30.953	1.870	33.993	1.00	141.76
	230	CD2	PHE	32 32	32.985	3.712	34.501	1.00	141.76
45		CE1	PHE	32 32	32.118	1.867	33.2 0 9		141.76
	232	CE2	PHE	32		2.787	33.464	1.00	141.76
	233	CZ	PHE PHE	32		4.481	37.408		141.76
	234	C	PHE	32		5.140	38.017		141.76 141.76
	235	0	GLU	33		4.055	37.969		141.76
50		N	GLU	33		4.330	39.369		141.76
	237	CA CB	GLU	33		3.831	40.292		141.76
	238	CG	GLU	33		2.332	40.223		141.76
	239 240	CD	GLU	33	27.251	1.496	40.519 40.92		141.76
5		OE1	GLU	33	26.216	2.073	40.92	·	141.76
3	242	OE2	GLU	33		0.256	39.68		141.76
	242	C	GLU	33		5.802	40.80		141.76
	244	ŏ	GLU	3		6.125	38.70		137.33
	245	Ň	VAL	3		6.689	38.89		137.33
6	0 246	CA	VAL	3			37.87		109.45
•	247	CB	VAL		4 27.428	40 444	37.97		109.45
	248	CG1			4 26.940		38.14		109.45
	249	CG2	VAL		4 28.929		38.63		
	250	С	VAL	3	4 25.167	0.207			

					04.000	8.503	39,545		137.33
	251	0	VAL		24.368	8.021	37.375	1.00	141.76
	252	N	SER	35	24.807	8.110	36.909	1.00	141.76
	253	CA	SER	35	23.432	9.522	36.351	1.00	133.69
	254 ·	CB	SER	35	23.189	9.652	35.667	1.00	133.69
	255	OG	SER	35	21.955	7.055	35.828	1.00	141.76
	256	C	SER	35	23.164	7.036	34.785	1.00	141.76
	257	0	SER	35	23.825 22.226	6.148	36.087	1.00	88.62
	258	N	SER	36	21.891	5.151	35.080	1.00	88.62
	259	CA	SER	36	20.818	4.198	35.591	1.00	92.65
10	260	CB	SER	36	19.623	4.905	35.850	1.00	92.65
10	261	OG	SER	36	21.335	6.012	33.959	1.00	88.62
	262	С	SER	36	20.928	7.150	34.193	1.00	88.62
	263	0	SER	36 37	21.332	5.495	32.741	1.00	66.50
	264	N	THR	37	20.833	6.279	31.625	1.00	66.50
15	265	CA	THR	37 37	21.718	6.049	30.395	1.00	64.10
_	266	CB	THR	37	23.085	6.313	30.748	1.00	64.10
	267	OG1	THR	37	21.299	6.969	29.254	1.00	64.10
	268	CG2	THR THR	37	19.369	6.003	31.268	1.00	66.50 66.50
	269	C	THR	37	18.855	4.912	31.478	1.00	59.63
20	270	0	LYS	38	18.693	7.025	30.764	1.00 1.00	59.63
	271	N	LYS	38	17.304	6.899	30.331		48.08
	272	CA CB	LYS	38	16.430	7.945	31.017	1.00 1.00	48.08
	273		LYS	38	15.696	7.418	32.220	1.00	48.08
~ ~	274	CD	LYS	38	15.075	8.535	33.017	1.00	48.08
25	275	CE	LYS	3ხ	14.471	7.971	34.289	1.00	48.08
	276	NZ	LYS	38	13.893	9.058	35.108 28.820	1.00	59.63
	277	C	LYS	38	17.274	7.120	28.343	1.00	59.63
	278 279	ŏ	LYS	38	17.770	8.140	28.068	1.00	49.53
30	280	N	TRP	39	16.719	6.166	26.599	1.00	49.53
30	281	CA	TRP	39	16.634	6.286	25.919	1.00	52.24
	282	CB	TRP	39	17.250	5.060 4.956	26.016	1.00	52.24
	283	CG	TRP	39	18.742	5.542	25.124	1.00	52.24
	284	CD2	TRP	39	19.701	5.189	25.598	1.00	52.24
35		CE2	TRP	39	20.985	6.338	23.972	1.00	52.24
55	286	CE3	TRP	39	19.601 19.461	4.288	26.966	1.00	52.24
	287	CD1	TRP	39	20.809	4.422	26.720	1.00	52.24
	288	NE1	TRP	39 39	22.158	5.601	24.961	1.00	52.24
	289	CZ2	TRP	39	20.772	6.750	23.339		52.24
40	290	CZ3	TRP	39	22.032	6.380	23.837		52.24
	291	CH2	TRP TRP	39		6.450	26.090		49.53 49.53
	292	C	TRP	39		5.831	26.608		52.82
	293	0	PHE	40		7.283	25.079		52.82
	294	N CA	PHE	40		7.470	24.529		55.71
45		CB	PHE	40		8.894	24.792 26.25		55.71
	296 297	CG	PHE	40	13.062	9.229	27.00		55.71
		CD1	PHE	40		9.497	26.90		55.71
	298 299	CD2	PHE	40) 11.833	9.208	28.36		55.71
5		CE1	PHE	40		9.719	28.28		
ر.	301	CE2	PHE	40		9.437 · 9.691	29.01		
	302	CZ	PHE	40		7.159	23.02		52.82
	303	C	PHE	41		7.133	22.22		52.82
	304	O	PHE	4		6.117	22.66		42.70
5	5 305	N	HIS	4		5.703	21.26		42.70
_	306	CA	HIS	4		4.176	21.18		48.50
	307	СВ	HIS		1 12.801		19.79		48.50
	308	CG	HIS		1 12.708 11 12.249		19.3		48.50
	309	CD2					18.6	98 1.00	
(60 310	ND1					17.6	04 1.00	
	311	CE1			11 12.931 11 12.397		17.9		
	312	NE2			41 11.408		20.8	42 1.0	
	313	Ç	HIS		41 10.387		21.4	34 1.0	0 42.70
	314	0	HIS	•	T, 10.50.				

	045	N	ASN	42 -	11.419	7.145	19.845	1.00	49.72
	315	CA	ASN	42	10.184	7.785	19.375	1.00	49.72
	316	CB	ASN	42	9.253	6.782	18.668	1.00	43.66
	317	CG .	ASN	42	9.743	6.393	17.280	1.00	43.66
_	318		ASN	42	10.632	7.053	16.729	1.00	43.66
5	319	OD1		42	9.156	5.340	16.708	1.00	43.66
	320	ND2	ASN	42	9.447	8.391	20.562	1.00	49.72
	321	C	ASN		8.220	8.372	20.609	1.00	49.72
	322	0	ASN	42	10.202	8.901	21.533	1.00	60.04
	323	N	GLY	43		9.505	22.706	1.00	60.04
10	324	CA	GLY	43	9.588	8.539	23.778	1.00	60.04
	325	C	GLY	43	9.100	8.961	24.748	1.00	60.04
	326	0	GLY	43	8.465		23.615	1.00	55.75
	327	N	SER	44	9.377	7.247	24.592	1.00	55.75
	328	CA	SER	44	8.948	6.249	23.908	1.00	71.51
15	329	CB	SER	44	8.280	5.058			71.51
	330	OG	SER	44	6.988	5.397	23.456	1.00 1.00	55.75
	331	С	SER	44	10.118	5.744	25.405		55.75 55.75
	332	0	SER	44	11.122	5.289	24.855	1.00	
	333	N	LEU	45	9.981	5.821	26.723	1.00	58.69
20	334	CA	LEU	45	11.040	5.380	27.609	1.00	58.69
	335	CB	LEU	45	10.639	5.585	29.068	1.00	58.46
	336	CG	LEU	45	11.647	5.140	30.129	1.00	58.46
	337	CD1	LEU	45	12.963	5.906	30.005	1.00	58.46
	338	CD2	LEU	45	11.017	5.358	31.491	1.00	58.46
25	339	С	LEU	45	11.375	3.925	27.366	1.00	58.69
	340	0	LEU	45	10.508	3.054	27.398	1.00	58.69
	341	N	SER	46	12.650	3.677	27.116	1.00	59.18
	342	CA	SER	46	13.138	2.336	26.B64	1.00	59.18
	343	CB	SER	46	14.437	2.402	26.077	1.00	54.40
30	344	OG	SER	46	15.025	1.120	26.000	1.00	54.40
•	345	С	SER	46	13.388	1.591	28.165	1.00	59.18
	346	Ö	SER	46	13.461	2.192	29.236	1.00	59.18
	347	Ñ	GLU	47	13.507	0.274	28.073	1.00	69.21
	348	CA	GLU	47	13.785	-0.524	29.252	1.00	69.21
35	349	СВ	GLU	47	13.256	-1.944	29.080	1.00	88.33
-	350	CG	GLU	47	11.752	-2.050	29.190	1.00	88.33
	351	CD	GLU	47	11.284	-3.483	29.278	1.00	88.33
	352	OE1	GLU	47	11.349	-4.198	28.256	1.00	88.33
	353	OE2	GLU	47	10.860	-3.898	30.377	1.00	88.33
40	354	Č	GLU	47	15.297	-0.541	29.433	1.00	69.21
	355	Ö	GLU	47	15.807	-0.973	30.462	1.00	69.21
	356	Ň	GLU	48	16.003	-0.057	28.415	1.00	63.82
	357	CA	GLU	48	17.456	0.011	28.433	1,00	63.82
	358	CB	GLU	48	17.980	0.306	27.025	1.00	75.50
45	359	CG	GLU	48	19.483	0.478	26.950	1.00	75.50
15	360	CD	GLU	48	20.223	-0.738	27.466	1.00	75.50
	361	OE1	GLU	48	20.152	-1.802	26.810	1.00	75.50
	362	OE2	GLU	48	20.863	-0.628	28.534	1.00	75.50
	363	č	GLU	48	17.902	1.113	29.394	1.00	63.82
50	364	ŏ	GLU	48	17.454	2.255	29.284	1.00	63.82
50	365	Ň	THR	49	18.792	0.772	30.322	1.00	72.39
	366	CA	THR	49	19.275	1.737	31.303	1.00	72.39
	367	CB	THR	49	18.867	1.316	32.727	1.00	60.69
	368	OG1	THR	49	19.140	-0.079	32.907	1.00	60.69
55	369	CG2	THR	49	17.381	1.573	32.953	1.00	60.69
33	370	C	THR	49	20.780	2.007	31.294	1.00	72.39
	371	ŏ	THR	49	21.247	2.896	31.998	1.00	72.39
	371	Ň	ASN	50	21.543	1.251	30.509	1.00	68.99
		CA	ASN	50	22.991	1.473	30.445	1.00	68.99
60	373	CB	ASN	50	23.710	0.247	29.879	1.00	96.77
OU			ASN	50	23.508	-0.989	30.733	1.00	96.77
	375	CG		50 50	23.625	-0.933	31.956	1.00	96.77
	376	OD1	ASN	50 50	23.209	-2.114	30.092	1.00	96.77
	377	ND2	ASN			2.693	29.579	1.00	68.99
	378	С	ASN	50	23.294	۵.053	23.013	1.00	50.33

	379 380	O N	ASN SER	51	22.424 24.527 24.927	3.178 3.186 4.369	28.856 29.655 28.892	1.00 1.00 1.00	68.99 51.99 51.99
	381	CA	SER	51 51	24.92 <i>1</i> 26.304	4.843	29.349	1.00	64.53
	382	CB	SER SER	51	27.281	3.878	28.998	1.00	64.53
	383	og	SER	51	24.978	4.074	27.391	1.00	51.99 51.99
	384	CO	SER	51	25.024	4.987	26. 56 9	1.00 1.00	68.17
	385 386	N	SER	52	24.998	2.793	27.045 25.650	1.00	68.17
	387	CA	SER	52	25.555	2.395 1.690	25.346	1.00	64.58
10	388	CB	SER	52	26.351 27.361	2.655	25.123	1.00	64.58
	389	OG	SER	52 52	23.866	1.502	25.248	1.00	68.17
	390	C	SER SER	52 52	23.621	0.468	25.864	1.00	68.17
	391	O N	LEU	53	23.136	1.927	24.221	1.00 1.00	42.59 42.59
15	392	CA	LEU	53	22.001	1.160	23.704 23.328	1.00	56.84
15	393 394	CB	LEU	53	20.856	2.108 1.569	22.678	1.00	56.84
	395	CG	LEU	53	19.581	0.285	23.349	1.00	56.84
	396	CD1	LEU	53	19.134 18.501	2.627	22.801	1.00	56.84
	397	CD2	LEU	53 53	22.4J4	0.407	22.473	1.00	42.59
20	398	C	LEU LEU	53	23.049	1.009	21.545	1.00	42.59 55.75
	399	O N	ASN	54	22.330	-0.911	22,479	1.00 1.00	55.75 55.75
	400 401	CA	ASN	54	22.762	-1.722	21.349 21.820	1.00	73.05
	402	CB	ASN	54	23.530	-2.950 -2.613	22.300	1.00	73.05
25	403	CG	ASN	54	24.921 25.717	-2.024	21.565	1.00	73.05
	404	OD1	ASN	54 54	25.717 25.225	-2.984	23.539	1.00	73.05
	405	ND2	ASN ASN	5 4 54	21.592	-2.177	20.493	1.00	55.75 55.75
	406	C O	ASN	54	20.643	-2.806	20.979	1.00 1.00	67.23
20	407 408	N	ILE	55	21.660	-1.835	19.212 18.281	1.00	67.23
30	408 409	CA	ILE	55	20.623	-2.237 -1.098	17.338	1.00	49.71
	410	CB	ILE	55	20.258 19.3 9 0	-1.096 -1.625	16.199	1.00	49.71
	411	CG2	ILE	55 55	19.550	-0.026	18.124	1.00	49.71
	412	CG1	ILE	55	19.172	1.189	17.333	1.00	49.71
35	413	CD1	ILE ILE	5 5	21.209	-3.398	17.498	1.00	67.23 67.23
	414	CO	ILE	55	22.197	-3.231	16.776 17.674	1.00 1.00	59.54
	415 · 416	Ň	VAL	56	20.618	-4.576 5.774	16.993	1.00	59.54
	417	CA	VAL	56	21.101	-5.774 -6.907	18.013	1.00	69.51
40		CB	VAL	56	21.340 21.949	-8.114	17.311	1.00	69.51
	419	CG1	VAL	56 56	22.262	-6.419	19.125		69.51
	420	CG2	VAL VAL	56	20.152	-6.270	15.898		59.54 59.54
	421	C O	VAL	56	18.932	-6.289	16.086		58.29
45	422 423	Ň	ASN	57	20.716	-6.684	14.763 13.618		58.29
45	423 424	CA	ASN	57	19.932	-7.171 -8.588	13.869		80.36
	425	СВ	ASN	57	19.399 20.503	-9.631	13.901		80.36
	426	CG	ASN	57		-9.723	12.97		80.36
	427	OD1	ASN	57 57		-10.428	14.96		80.36 58.29
50		ND2	ASN ASN	57		<i>-</i> 6.195	13.43		58.29
	429	CO	ASN	57		-6.517	13.66		46.57
	430 431	Ň	ALA	58	19.166	-4.991	13.02 12.84		46.57
	432	CA	ALA	58		-3.885 -2.774	12.07		27.34
5	5 433	СВ	ALA	58		-4.227	12.17	0 1.00	46.57
Ū	434	C	ALA	58 58		-4.920	11.14	1 1.00	46.57
	435	0	ALA LYS	59		-3.732	12.73		53.79 53.79
	436	N CA	LYS	59	14.520	-3.949	12.14		53.79 70.29
_	437 50 438	CB	LYS	5	9 13.543	-4.514	13.16 13.91		70.29
C	439	CG	LYS	5		-5.733 -5.989	15.11		70.29
	440	CD	LYS	5		-5.869	16.03		70.29
	441	CE	LYS		9 13.770 9 12.856		17.18		70.29
	442	NZ	LYS	5	3 12.000	•			

	443	C	LYS LYS	59 · 59	14.033 14.593	-2.579 -1.549	11.682 12.062	1.00 1.00	53.79 53.79
	444	0 N	PHE	60	13.011	-2.563	10.839	1.00 1.00	57.14 57.14
	445 446	CA	PHE	60	12.473	-1.301	10.359 9.355	1.00	75.29
	447	СВ	PHE	60	11.350	-1.549 -2.022	8.019	1.00	75.29
	448	CG	PHE	60 60	11.823 11.028	-2.876	7.259	1.00	75.29
	449	CD1	PHE PHE	60	13.043	-1.596	7.499	1.00	75.29
	450	CD2 CE1	PHE	60	11.437	-3.304	5.999	1.00 1.00	75.29 75.29
10	451	CE2	PHE	60	13.465	-2.016	6.237 5.485	1.00	75.29
10	452 453	CZ	PHE	60	12.657	-2.873 -0.568	11.567	1.00	57.14
	454	С	PHE	60	11.922	0.659	11.609	1.00	57.14
	455	0	PHE	60 61	11.895 11.484	-1.345	12.550	1.00	62.19
	456	N	GLU GLU	61	10.921	-0.803	13.778	1.00	62.19
15	457	CA CB	GLU	61	10.401	-1.937	14.671	1.00	93,34 93.34
	458 459	CG	GLU	61	9.199	-2.699	14.121 12.827	1.00 1.00	93.34
	459 460	CD	GLU	61	9.496	-3.449 -4.2 8 5	12.815	1.00	93.34
	461	OE1	GLU	61	10.425 8.792	-3.203	11.823	1.00	93.34
20	462	OE2	GLU	61 61	11.960	0.013	14.552	1.00	62.19
	463	C	GLU GLU	61	11.609	0.932	15.285	1.00	62.19 48.05
	464	O N	ASP	62	13.235	-0.315	14.384	1.00 1.00	48.05 48.05
	465 466	CA	ASP	62	14.272	0.406	15.107 15.119	1.00	36.56
25	467	CB	ASP	62	15.573	-0.389 -1.725	15.809	1.00	36.56
23	468	CG	ASP	62	15.420 14.696	-1.799	16.822	1.00	36.56
	469	OD1	ASP	62 62	16.025	-2.703	15.355	1.00	36.56
	470	OD2	ASP ASP	62	14.516	1.790	14.535	1.00	48.05 48.05
20	471	C O	ASP	62	15.250	2.587	15.110 13.399	1.00 1.00	39.66
30	472 473	Ň	SER	63	13.896	2.076 3.386	12.809	1.00	39.66
	474	CA	SER	63	14.076	3.454	11.428	1.00	51.20
	475	CB	SER	63	13.420 14.091	2.604	10.524	1.00	51.20
	476	OG	SER SER	63 63	13.419	4.361	13.759	1.00	39.66
35	477	O .	SER	63	12.647	3.966	14.630	1.00 1.00	39.66 35.00
	478 479	N	GLY	64	13.722	5.637	13.613 14.521	1.00	35.00
	480	CA	GLY	64	13.108	6.589 7.568	15.260	1.00	35.00
	481	С	GLY	64	14.014 15.207	7.696	14.975	1.00	35.00
40	482	0	GLY GLU	64 65	13.406	8.261	16.214	1.00	46.87
	483	N	GLU	65	14.075	9.259	17.020		46.87 64.86
	484 485	CA CB	GLU	65	13.101	10.390	17.340 18.222		64.86
	485 486	CG	GLU	65	13.685	11.460 12.430	18.727		64.86
45		CD	GLU	65	12.647 11.819	12.430	19.574		64.86
	488	OE1	GLU	65 65		13.596	18.274	1.00	64.86
	489	OE2	GLU	65		8.683	18.327		46.87 46.87
	490	CO	GLU	65		7.988	19.046		50.39
50	491 0 492	Ň	TYR	66	15.845	8.985	18.632 19.882		50.39
)(493	CA	TYR	66		8.533 7.535	19.60		40.76
	494	CB	7.79	66		6.188	19.14	3 1.00	40.76
	495	CG	TYR	66 66		5.843	17.80		40.76
	496	CD1 CE1	TYR TYR	66		4.585	17.38		40.76 40.76
5	5 497	CD2		6	6 16.652	5.236	20.05 19.64		40.76
	498 499	CE2		6		3.973	18.31		40.76
	500	CZ	TYR	6		3.653 2.378	17.91		40.76
	501	OH	TYR	6		9.711	20.65	8 1.00	50.39
(50 502	Ç	TYR TYR		6 17.032 6 17.732		20.07	75 1.00	50.39 55.49
	503	O N	LYS		7 16.719	9.785	21.95		
	504 505	CA	LYS	6	7 17.221	10.837	22.85 23.37		
	505 506	CB	LYS	E	37 16.106	11.762	20.0	, , , , , , ,	•
	3								

									•
	507	CG	LYS	67 ·	15.118	12.362	22.412	1.00	68.70
	507	CD	LYS	67	13.879	12.767	23.199	1.00	68.70
	508 509	CE	LYS	67	12.818	13.407	22.338	1.00	68.70
	510°	NZ	LYS	67	11.597	13.688	23.149	1.00	68.70
5	511	C	LYS	67	17.734	10.114	24.092	1.00	55.49
•	512	0	LYS	67	17.209	9.054	24.446	1.00	55.49
	513	N	CYS	68	18.749	10.658	24.759	1.00	60.89
	514	CA	CYS	68	19.179	10.011	25.992 27.145	1.00 1.00	60.89 60.89
	515	Ç	CYS	68	19.028	10.988 12.193	27.145 26. 94 6	1.00	60.89
10	516	0_	CYS	68	18.795 20.594	9.418	25.897	1.00	63.38
	517	CB	CYS	68 68	22.069	10.482	25.959	1.00	63.38
	518	SG	CYS GLN	69	19.113	10.457	28.355	1.00	61.40
	519	N CA	GLN	69	18.943	11.268	29.546	1.00	61.40
15	520 521	CB	GLN	69	17.495	11.161	29. 99 8	1.00	108.41
13	522	CG	GLN	69	17.207	11.587	31.426	1.00	108.41
	523	CD	GLN	69	16.245	12.754	31.486	1.00	108.41
	524	OE1	GLN	69	15.641	13.126	30.493	1.00	108.41
	525	NE2	GLN	69	16.097	13.333	32.665	1.00	108.41
20	526	С	GLN	69	19.858	10.792	30.642	1.00 1.00	61.40 61.40
	527	0	GLN	69	19.859	9.609	31.005	1.00	103.97
	528	N	HIS	70	20.653	11.729 11.480	31.139 32.217	1.00	103.97
	529	CA	HIS	70 70	21.594 23.011	11.824	31.761	1.00	140.89
25	530	CB	HIS HIS	70 70	24.032	11.697	32.844	1.00	140.89
25	531	CG CD2	HIS	70	24.744	12.638	33.503	1.00	140.89
	532 533	ND1	HIS	70	24.407	10.485	33.376	1.00	140.89
	534	CE1	HIS	70	25.311	10.685	34.319	1.00	140.89
	535	NE2	HIS	70	25.534	11.984	34.416	1.00	140.89
30	536	C	HIS	70	21.186	12.373	33.396	1.00	103.97
	537	0	HIS	70	20.184	13.088	33.319	1.00	103.97 101.70
	538	N	GLN	71	21.968	12.364	34.470 35.640	1.00 1.00	101.70
	539	CA	GLN	71	21.646	13.1 6 3 12.706	36. 82 0	1.00	136.43
25	540	CB	GLN	71 71	22.512 21. 73 9	11.968	37. 9 24	1.00	136.43
35	541	CG	GLN GLN	71	22.639	11.194	38.876	1.00	136.43
	542	CD OE1	GLN	71	23.660	11.696	39.322	1.00	136.43
	543 544	NE2	GLN	71	22.242	9.966	39.206	1.00	136.43
	5 4.5	.C	GLN	71	21.782	14.663	35.407	1.00	101.70
40	546	Ö	GLN	71	21.838	15.441	36.361	1.00	101.70
10	547	N	GLN	72	21.778	15.065	34.137	1.00	141.76
	548	CA	GLN	72	21.905	16.470	33.755	1.00	141.76
	549	CB	GLN	72	22.748	16.587	32.494	1.00	141.59 141.59
	550	CG	GLN	72	24.182	16.131 16.307	32.710 31.482	1.00 1.00	141.59
45	551	CD	GLN	72	25.045 24.616	16.858	30.472	1.00	141.59
	552	OE1	GLN	72 72	26.285	15.841	31.570	1.00	141.59
	553	NE2	GLN GLN	72	20.578	17.187	33.541	1.00	141.76
	554 555	C O	GLN	72	20.531	18.246	32.918	1.00	141.76
50	556	Ň	VAL	73	19.509	16.598	34.067	1.00	141.76
50	557	.CA	VAL	73	18.150	17.144	33.996	1.00	141.76
	558	CB	VAL	73	17.945	18.230	35.093	1.00	113.45
	559	CG1	VAL	73	16.471	18.593	35.215	1.00	113.45
	560	CG2	VAL	73	18.475	17.718	36.424	1.00	113.45
55	561	C	VAL	73	17.677	17.707	32.644	1.00	141.76 141.76
	562	0	VAL	73	16.643	18.376	32.568 31.583	1.00 1.00	110.03
	563	N	ASN	74 74	18.433	17.441 17.906	30.249	1.00	110.03
	564	CA	ASN	74 74	18.056 18.782	19.208	29.880	1.00	123.79
<i>(</i> 0	565	CB	ASN ASN	74 74	18.013	20,459	30.295	1.00	123.79
60	566 567	CG OD1	ASN	74	16.818	20.402	30.597	1.00	123.79
	567 568	ND2	ASN	74	18.698	21.598	30.291	1.00	123.79
	569	C	ASN	74	18.382	16.840	29.212	1.00	110.03
	570	ŏ	ASN	74	19.531	16.412	29.094	1.00	110.03

			CLLI	75 ·	17.367	16.416	28.460	1.00	64.12
	571	N CA	GLU GLU	75 75	17.552	15.399	27.433	1.00	64.12
	572 573	CB	GLU	75	16.190	14.961	26.882	1.00	93.37
	574	CG	GLU	75	15.332	14.330	27.971	1.00	93.37
5	575	CD	GLU	75	13.963	13.868	27.511	1.00	93.37
•	576	OE1	GLU	75	13.583	14.146	26.355	1.00	93.37
	577	OE2	GLU	75	13.264	13.227	28.327	1.00	93.37
	578	С	GLU	75	18.454	15.910	26.319	1.00	64.12
	579	0	GLU	75	18.591	17.118 14.984	26.120 25.611	1.00 1.00	64.12 56.18
10	580	N	SER	76 76	19.0 9 0 19.980	15.362	24.518	1.00	56.18
	581	CA	SER SER	76 76	20.944	14.217	24.188	1.00	74.86
	582	CB OG	SER	76	20.235	13.084	23.720	1.00	74.86
	583 584	C	SER	76	19.189	15.720	23.263	1.00	56.18
15	585	ŏ	SER	76	17.968	15.559	23.199	1.00	56.18
13	586	Ň	GLU	77	19.896	16.237	22.271	1.00	67.41
	587	CA	GLU	77	19.250	16.561	21.021	1.00	67.41
	588	СВ	GLU	77	20.205	17.326	20.096	1.00	96.50
	589	CG	GLU	77	20.530	18.734	20.563 20.859	1.00 1.00	96.50 96.50
20	590	CD	GLU	77	19.281	19.545 19.638	19.973	1.00	96.50
	591	OE1	GLU GLU	77 77	18.406 19.173	20.089	21.978	1.00	96.50
	592	OE2	GLU	77	18.903	15.205	20.416	1.00	67.41
	593 594	C	GLU	77	19.605	14.210	20.646	1.00	67.41
25	595	Ň	PRO	78	7.805	15.136	19.660	1.00	64.74
23	596	CD	PRO	78	16.712	16.106	19.495	1.00	62.17
	597	CA	PRO	78	17.447	13.852	19.067	1.00	64.74
	598	CB	PRO	78	16.047	14.101	18.514	1.00	62.17 62.17
	599	CG	PRO	78	15.527	15.197	19.372 17.959	1.00 1.00	64.74
30	600	Ç	PRO	78 70	18.421 19.118	13.473 14.321	17.404	1.00	64.74
	601	0	PRO VAL	78 79	18.469	12,183	17.670	1.00	45.82
	602	N CA	VAL	79	19.274	11.638	16.593	1.00	45.82
	603 604	CB	VAL	79	20.455	10.798	17.123	1.00	63.76
35	605	CG1	VAL	79	21.165	10.108	15.972	1.00	63.76
33	606	CG2	VAL	79	21.437	11.702	17.841	1.00	63.76
	607	C	VAL	79	18.266	10.745	15.857	1.00	45.82
	608	0	VAL.	79	17.396	10.128	16.485	1.00 1.00	45.82 52.05
	609	N	TYR	80	18.347	10.697 9.886	14.533 13.790	1.00	52.05
40	610	CA	TYR	80 80	17.396 16.612	10.760	12.810	1.00	70.93
	611	CB CG	TYR TYR	80	15.767	11.787	13.520	1.00	70.93
	612 613	CD1	TYR	80	16.329	12.975	13.998	1.00	70.93
	614	CE1	TYR	80	15.573	13.882	14.744	1.00	70.93
45		CD2	TYR	80	14.422	11.533	13.798	1.00	70.93
	616	CE2	TYR	80	13.656	12.427	14.543	1.00	70.93
	617	CZ	TYR	80	14.237	13.598	15.017	1.00	70.93 70.93
	618	OH	TYR	80	13.493	14.459	15.798 13.074	1.00 1.00	52.05
~^	619	Ç	TYR	80	18.016 18.975	8.711 8.859	12.320	1.00	52.05
50		0	TYR LEU	80 81	17.464	7.532	13.332	1.00	46.77
	621	N CA	LEU	81	17.960	6.319	12.702	1.00	46.77
	622 623	CB	LEU	81	18.213	5.249	13.767	1.00	49.82
	624	CG	LEU	81	19.042	4.032	13.338	1.00	49.82
55	625	CD1	LEU	81	20.515	4.427	13.231	1.00	49.82
	626	CD2	LEU	81	18.884	2.907	14.354	1.00	49.82 46.77
	627	С	LEU	81	16.935	5.811	11.659 11.881	1.00 1.00	46.77 46.77
	628	0	LEU	81	15.720	5.865 5.337	10.523	1.00	44.84
-	629	N	GLU	82 82	17.434 16.568	4.816	9.487	1.00	44.84
60		CA	GLU GLU	82	16.372	5.863	8.395	1.00	75.78
	631 632	CB CG	GLU	82	15.459	5.412	7.277	1.00	75.78
	633	CD	GLU	82	14.890	6.571	6.490	1.00	75.78
	634	OE1	GLU	82	15.573	7.613	6.387	1.00	75.78

	635	OE2	GLU	82 .	13.764	6.437 3.526		1.00 1.00	75.78 44.84
	636	С	GLU	82	17.124	3.478		1.00	44.84
	637	0	GLU	82	18.256 16.308	2.482		1.00	58.13
_	638	N	VAL VAL	83 83	16.715	1.177		1.00	58.13
5	639	CA	VAL	83	16.204	0.070		1.00	48.46
	640	CB CG1	VAL	83	16.693	-1.285		1.00	48.46
	641 642	CG2	VAL	83	16.668	0.369		1.00	48.46 58.13
	643	C	VAL	83	16.212	0.919	6.986 6.697	1.00 1.00	58.13
10	644	ŏ	VAL	83	15.033	1.088	6.103	1.00	54.77
10	645	N	PHE	84	17.118	0.509 0.235	4.720	1.00	54.77
	646	CA	PHE	84	16.772 17.572	1.115	3.750	1.00	54.95
	647	СВ	PHE	84 84	17.424	2.584	3.986	1.00	54.95
	648	CG	PHE PHE	84	18.222	3.227	4.937	1.00	54.95
15	649	CD1 CD2	PHE	84	16.503	3.336	3.246	1.00	54.95
	650 651	CE1	PHE	84	18.111	4.600	5.143	1.00	54.95 54.95
	652	CE2	PHE	84	16.378	4.708	3.438 4.388	1.00 1.00	54.95
	653	CZ	PHE	84	17.185	5.349 -1.194	4.305 4.305	1.00	54.77
20	654	С	PHE	84	17.031	-1.194 -1.947	4.980	1.00	54.77
	655	0	PHE	84	17.743 16.474	-1.527	3.148	1.00	50.72
	656	N	SER	85 85	16.625	-2.831	2.519	1.00	50.72
	657	CA	SER SER	85	15.392	-3.696	2.776	1.00	85.41
0.5	658	CB OG	SER	85	15.578	-4.996	2.253	1.00	85.41
25	659 660	C	SER	85	16.737	-2.509	1.031	1.00 1.00	50.72 50.72
	661	ŏ	SER	85	15.741	-2.166	0.397 0.470	1.00	46.74
	662	N	ASP	86	17.933	-2.595 -2.283	-0.939	1.00	46.74
	663	CA	ASP	86	18.122	-2.265 -0.766	-1.139	1.00	57.20
30	664	CB	ASP	86	18.070 17.810	-0.345	-2.581	1.00	57.20
	665	CG	ASP ASP	86 86	18.547	-0.781	-3.500	1.00	57.20
	666	OD1 OD2	ASP	86	16.866	0.442	-2.795	1.00	57.20
	667	C	ASP	86	19.499	-2.821	-1.277	1.00	46.74 46.74
35	668 669	ŏ	ASP	86	20.166	-3.402	-0.429	1.00 1.00	48.74 48.74
33	670	Ň	TRP	87	19.936	-2.615	-2.505 -2.935	1.00	48.74
	671	CA	TRP	87	21.241	-3.073 -3. 36 6	-4.440	1.00	51.62
	672	CB	TRP	87 97	21.226 20.649	-4.704	-4.804	1.00	51.62
	673	CG	TRP	87 87	19.258	-5.039	-4.934	1.00	51.62
40	674	CD2 CE2	TRP TRP	87	19.191	-6.406	-5.285	1.00	51.62
	675 676	CE3	TRP	87	18.064	-4.316	-4.793	1.00	51.62 51.62
	676 677	CD1	TRP	87	21.344	-5.846	-5.072	1.00 1.00	51.62
	678	NE1	TRP	87	20.479	-6.872	-5. 3 61 -5. 50 0	1.00	51.62
45	679	CZ2	TRP	87	17.966	-7.069 -4.974	-5.006	1.00	51.62
-	680	CZ3	TRP	87	16.849 16.813	-6.337	-5.357	1.00	51.62
	681	CH2	TRP	87 87	22.285	-2.011	-2.634	1.00	48.74
	682	C	TRP TRP	87	23.440	-2.327	-2.297	1.00	48.74
50	683) 684	N	LEU	88	21.889	-0.752	-2.793	1.00	48.62 48.62
30	685	ČA	LEU	88	22.774	0.361	-2.517	1.00 1.00	41.58
	686	CB	LEU	88		1.159 0.628	-3.775 -4.731	1.00	41.58
	687	CG	LEU	88		1.715	-5.724	1.00	41.58
	688	CD1	LEU	88		0.208	-3.975	1.00	41.58
5:		CD2	LEU	· 88		1.290	-1.503	1.00	48.62
	690	C	LEU	88		1.448	-1.458		48.62
	691	O N	LEU	89		1.895	-0.683		46.32
	692 693	CA	LEU	89	22,532	2.823	0.336		46.32 41.30
6		CB	LEU	89		2.098	1.671 2.913		41.30
J	695	CG	LEU	89		2.940	2.656		41.30
	696	CD1	LEU	89		3.782 2.032	4.113		41.30
	697	CD2	LEU	89			0.459		46.32
	698	С	LEU	8	23.000	0.000			

•	699 700 701	O N CA	LEU LEU LEU	89 - 90 90	24.821 23.259 24.233	3.509 5.134 6.196 7.418	0.353 0.489	1.00 1.00 1.00 1.00	46.32 43.08 43.08 46.82
5	702 703 704 705	CB CG CD1 CD2	LEU LEU LEU	90 90 90	23.818 24.810 26.217 24.344	8.588 8.116 9.655	-0.299 -0.656 -1.270	1.00 1.00 1.00 1.00	46.82 46.82 46.82 43.08
	706 707 708 709	C O N CA	LEU LEU GLN GLN	90 90 91 91	24.229 23.177 25.404 25.484	6.528 6.760 6.493 6.817	2.571	1.00 1.00 1.00 1.00	43.08 44.37 44.37 39.09
15	710 711 712 713	CB CG CD OE1	GLN GLN GLN GLN	91 91 91 91	26.177 25.435 26.190 27.337	5.695 4.377 3.286 2.992	4.730 5.468 5.162 6.433	1.00 1.00 1.00 1.00	39.09 39.09 39.09 39.09
13	714 715 716	NE2 C O N	GLN GLN GLN ALA	91 91 91 92	25.535 26.261 27.172 * 25.860	2.678 8.121 8.390 8.948	4.136 3.357 5.091	1.00 1.00 1.00	44.37 44.37 44.40 44.40
20	717 718 719 720	CA CB C	ALA ALA ALA ALA	92 92 92 92	26.534 25.618 26.921 26.223	10.217 11.365 10.332 9.806	5.309 4.952 6.767 7.631	1.00 1.00 1.00 1.00	35.90 44.40 44.40
25	721 722 723 724	O N CA CB	SER SER SER SER	93 93 93 93	28.025 28.435 29.821 29.947	11.019 11.214 11.866 12.998	7.041 8.419 8.493 7.649	1.00 1.00 1.00 1.00	39.65 39.65 42.29 42.29
30	725 726 727 728	OG C O N	SER SER ALA	93 93 94 94	27.373 27.048 26.801 25.759	12.092 11.939 13.006 13.865	9.062 10.239 8.291 8.848	1.00 1.00 1.00 1.00	39.65 39.65 49.05 49.05
	729 730 731 732	CA CB C O	ALA ALA ALA	94 94 94	26.397 24.815 25.238 23.542	15.014 14.416 14.702 14.563	9.617 7.775 6.668 8.099	1.00 1.00 1.00 1.00	25.45 49.05 49.05 54.30
35	733 734 735 736	N CA CB CG	GLU GLU GLU GLU	95 95 95 95	22.598 21.200 21.107	15.115 14.552 13.088 12.488	7.126 7.355 6.999 7.345	1.00 1.00 1.00 1.00	54.30 64.16 64.16 64.16
40	737 738 739 740	CD OE1 OE2 C	GLU GLU GLU	95 95 95 95	19.770 19.563 18.926 22.594	11.286 13.218 16.636	7.063 7.899 7.253 6.405	1.00 1.00 1.00 1.00	64.16 64.16 54.30 54.30
45	741 742	O N CA CB	GLU VAL VAL VAL	95 96 96 96	22.044 23.234 23.366 22.414	17.332 17.127 18.550 19.000	8.317 8.595 9.707	1.00 1.00 1.00	54.64 54.64 44.67 44.67
50	745 746 747	CG1 CG2 C	VAL VAL VAL VAL	96 96 96 96	24. 80 0 25.161	20.472 18.784 18.787 18.494	10.030 9.274 9.049 10.194	1.00 1.00 1.00	44.67 54.64 54.64 48.96
30	749 750 751	N CA CB	VAL VAL VAL VAL	97 97 97 97	25.613 27.023 27.866	19.306 19.592 19.209 19.450	8.134 8.365 7.133 7.407	1.00 1.00 1.00 1.00	48.96 46.14 46.14
55	754 755	CG1 CG2 C	VAL VAL VAL	97 97 97 98	27.628 27.257 26.654	17.773 21.078 21.934 21.385	6.764 8.619 7.956 9.560	1.00 1.00 1.00 1.00	46.14 48.96 48.96 48.67
60	759	N CA CB CG	MET	98 98 98	28.479 28.895 27.724	22.770 22.920 22.792 23.133	9.866 11.329 12.290 14.001	1.00 1.00	48.67 88.16 88.16 88.16
	760 761 762	SD CE C	MET MET MET	9(9) 9)	8 28.281	21.471 23.222	14.634 8.937	1.00	88.16 48.67

					00.407	22,451	8.603	1.00	48.67
76	3	0	141-		30.487	24.467	8.488	1.00	51.28
76		N	GLU	99	29.516	25.003	7.579	1.00	51.28
76		CA	GLU	99	30.518	26.488	7.339	1.00	66.75
76		ÇB	GLU	99	30.227	27.175	6.403	1.00	66.75
5 76		CG	GLU	99	31.195 30.842	28.632	6.164	1.00	66.75
76	68	CD	GLU	99	30.515	29.334	7.146	1.00	66.75
	69	OE1	GLU	99	30.901	29.072	4.994	1.00	66.75
	70	OE2	GLU	99 99	31.939	24.801	8.133	1.00	51.28
	71	С	GLU	99	32.182	25.000	9.318	1.00	51.28
10 7	72	0	GLU	100	32.874	24.401	7.280	1.00	56.63 56.63
	73	N	GLY	100	34.233	24.185	7.748	1.00	56.63
7	74	CA	GLY GLY	100	34.534	22.752	8.172	1.00	56.63
	75	C	GLY	100	35.670	22.300	8.074	1.00 1.00	64.74
7	776	0	GLN	101	33.519	22.037	8.654	1.00	64.74
	777	N CA	GLN	101	33.683	20.645	9.065 10.003	1.00	77.71
7	778	CB	GLN	101	32.550	20.236	11.325	1.00	77.71
	779 700	CG	GLN	101	32.559	20.959	12.090	1.00	77.71
	780 781	CD	GLN	101	33.844	20.719	11.702	1.00	77.71
	781 782	OE1	GLN	101	34.912	_1.200 19.957	13.179	1.00	77.71
	783	NE2	GLN	101	33.751	19.702	7.855	1.00	64.74
	784	C	GLN	101	33.695	20.083	6.745	1.00	64.74
	785	Ō	GLN	101	33.327	18.452	8.055	1.00	53.53
	786	N	PRO	102	34.132	17.877	9.236	1.00	44.31
25	787	CD	PRO	102	34.809 34.163	17.510	6.936	1.00	53.53
20	788	CA	PRO	102	35.317	16.590	7.311	1.00	44.31
	789	CB	PRO	102 102	35.0 9 7	16.438	8.790	1.00	44.31
	790	CG	PRO	102		16.752	6.795	1.00	53.53
	791	C	PRO	102		16.635	7.739	1.00	53.53 42.44
30	792	0	PRO LEU	103		16.242	5.596	1.00	42.44
	793	N	LEU	103		15.480	5.300	1.00 1.00	43.14
	794	CA	LEU	103		16.243	4.317		43.14
	795	CB CG	LEU	103	29.332	15.406	3.768 4.920		43.14
25	79 6	CD1	LEU	103	28.454	14.974	2.768		43.14
35	797 709	CD2	LEU	103	28.522	16.193	4.673		42.44
	798 799	C	LEU	103		14.169	3.679		42.44
	800	ŏ	LEU	103		14.163 13.052	5.246		40.42
	801	N	PHE	10-		11.772	4.659		40.42
40	802	CA	PHE	10			5.701	1.00	57.95
40	803	СВ	PHE	10		11.515	6.453	3 1.00	57.95
	804	ÇG	PHE	10			7.62		57.95
	805	CD1	PHE	10 10			6.00		57.95
	806	CD2	PHE	10		12.836	8.34		57.95 57.95
45	807	CE1	PHE PHE	10			6.71		57.95 57.95
	808	CE2	PHE	10		12.721	7.88		40.42
	809	CZ	PHE		30.63	5 11.025	4.04		40.42
	810	C	PHE		29.57	10.900	4.66		44.12
50	811	N	LEU	10	05 30.83		2.83 2.14		44.12
50	812	CA	LEU	10	05 29.81		0.84		40.26
	813 814	CB	LEU		05 29.38		0.98		40.26
	815	ĊĠ	LEU		05 28.87		-0.30		40.26
	816	CD1	LEU		05 28.55		1.89		40.26
55	817	CD2	LEU		05 27.66		1.8		44.12
55	818	С	LEU		05 30.38 05 31.58		1.6		44.12
	819	0	LEU				1.7	45 1.00	45.34
	820	N	ARG				1.4	84 1.00	45.34
	821	CA	ARG		106 29.91 106 30.13		2.8		
60	822	CB	ARG		106 30.59	4	2.8		
	823	CG	ARG ARG		106 30.2	3.378		62 1.00	
	824	CD	ARG		106 30.8	88 2.066		356 1.00	
	825	NE CZ	ARG		106 30.5		5.2	297 1.00	37.54
	826	CZ	And						

			4 520	6.128 1.00	57.54
827	NH1 ARG	106 · 29.516	1.530 0.040	5.407 1.00	57.54
828	NH2 ARG	106 31.110 106 28.800	5.359	0.710 1.00	45.34
829	C ARG	106 28.800 106 27.658	5.345	1.160 1.00	45.34
830	O ARG N CYS	107 29.129	4.824	-0.465 1.00	48.19
5 831	N CYS CA CYS	107 28.156	4.098	-1.275 1.00	48.19
832 833	C CYS	107 28.337	2.663	-0.779 1.00	48.19
834	o cys	107 29.268	1.948	-1.166 1.00 -2.769 1.00	48.19 54.03
835	CB CYS	107 28.474	4.238	-2.769 1.00 -3.893 1.00	54.03
10 836	SG CYS	107 27.089	3.836 2.286	0.116 1.00	52.57
837	N HIS	108 27.430 108 27.433	1.009	0.797 1.00	52.57
838	CA HIS	108 27.433 108 26.986	1.261	2.243 1.00	42.83
839	CB HIS	108 27.086	0.067	3.134 1.00	42.83
840	CG HIS CD2 HIS	108 26.211	-0.448	4.029 1.00	42.83
15 841 842	ND1 HIS	108 28.214	-0.725	3.196 1.00	42.83 42.83
843	CE1 HIS	108 28.026	-1.677	4.092 1.00 4.613 1.00	42.83 42.83
844	NE2 HIS	108 26.820	-1.531	4.613 1.00 0.136 1.00	52.57
845	C HIS	108 26.567	-0.048 0.192	-0.174 1.00	52.57
20 846	O HIS	108 25.398 109 27.144	-1.226	-0.072 1.00	46.92
. 847	N GLY	109 27.144 109 26.413	-2.313	-0.703 1.00	46.92
848	CA GLY C GLY	109 25.824	-3.310	0.273 1.00	46.92
849	C GLY O GLY	109 26.406	-3.596	1.309 1.00	46.92
850 25 851	N TRP	110 24.657	-3.840	-0.063 1.00	39.32 39.32
852	CA TRP	110 23.983	-4.832	0.771 1.00 -0.014 1.00	39.32 37.53
853	CB TRP	110 22.807	-5.430	-0.014 1.00 0.744 1.00	37.53
854	CG TRP	110 22.002	-6.428 -6.153	1.710 1.00	37.53
855	CD2 TRP	110 20.978 110 20.507	-7.399	2.183 1.00	37.53
30 856	CE2 TRP CE3 TRP	110 20.507 110 20.414	-4.973	2.225 1.00	37.53
857	CE3 TRP CD1 TRP	110 22.105	<i>-</i> 7.785	0.672 1.00	37.53
858 859	NE1 TRP	110 21.212	-8.376	1.531 1.00	37.53
860	CZ2 TRP	110 19.494	-7.508	3.152 1.00 3.195 1.00	37.53 37.53
35 861	CZ3 TRP	110 19.400	-5.078	3.195 1.00 3.645 1.00	37.53
862	CH2 TRP	110 18.954	-6.344 -5.918	1,134 1.00	39.32
863	C TRP	110 24.991 110 25.816	-6. 297	0.309 1.00	39.32
864	O TRP	110 25.816 111 24.938	-6.405	2.369 1.00	45.97
865	N ARG CA ARG	111 25.876	-7.447	2.818 1.00	45.97
40 866 867	CB ARG	111 25.607	-8.754	2.093 1.00	58.00
868	CG ARG	111 24.357	-9.430	2.525 1.00 1.934 1.00	58.00 58.00
869	CD ARG	111 24.273	-10.832	1.934 1.00 2.786 1.00	58.00
870	NE ARG	111 23.403	-11.623 -12.728	3.406 1.00	58.00
45 871	CZ ARG	111 23.773 111 25.005	-13.203	3.260 1.00	58.00
872	NH1 ARG		-13.322	4.218 1.00	58.00
873 874	NH2 ARG C ARG		-7.099	2.583 1.00	45.97
874 875	O ARG		-7.996	2.501 1.00	45.97 52.35
50 876	N ASN	112 27.645	-5.817	2.438 1.00 2.172 1.00	52.35
877	CA ASN		-5.420 5.706	2.172 1.00 3.341 1.00	76.11
878	CB ASN		-5.796 -4.718	4.374 1.00	76.11
879	CG ASN		-3.629	4.117 1.00	76.11
880	OD1 ASN ND2 ASN		-4.997	5.553 1.00	76.11
55 881	ND2 ASN C ASN		-6.010	0.883 1.00	52.35
882 883	o ASI	112 30.778	-6.304	0.792 1.00	52.35 53.59
884	N TRE	113 28.719	-6.180	-0.110 1.00 -1.386 1.00	53.59 53.59
885	CA TR		-6.682 -6.922	-2.333 1.00	53.83
60 886	CB TRI		-8.138	-1.993 1.00	53.83
887	CG TRI		-8.348	-2.273 1.00	
888	CD2 TRI		-9.634	-1.783 1.00	
889 89 0	CE3 TR		<i>-</i> 7.578	-2.895 1.00	53.83
650	020 111	•			

•								4.00	53.83
				113 -	27.607	-9.273	-1.368		
1	B91	V •	TRP	113	26.578	-10.173	-1.236		53.83
	892	• • •	TRP	113	24.144	-10.169	-1.888	1.00	53.83
	893		TRP	113	23.490	-8.107	-3.002	1.00	53.83
	894	CZ3	TRP		23.186	-9.394	-2.500	1.00	53.83
	895	CH2	TRP	113	30.068	-5.583	-1.939	1.00	53.59
	896	С	TRP	113	29.892	-4.407	-1.605	1.00	53.59
	897	0	TRP	113	31.022	-5.950	-2.779	1.00	64.92
	898	N	ASP	114		-4.950	-3.363	1.00	64.92
	899	CA	ASP	114	31.893	-5.602	-4.020	1.00	80.11
10	900	СВ	ASP	114	33.105	-6.427	-3.046	1.00	80.11
10	901	CG	ASP	114	33,906	-5.892	-1.968	1.00	80.11
		OD1	ASP	114	34.241	-7.603	-3.355	1.00	80.11
	902	OD2	ASP	114	34.195		-4.390	1.00	64.92
	903	C	ASP	114	31.122	-4.148 4.601	-5.170	1.00	64.92
	904	ŏ	ASP	114	30.332	-4.691	-4.375	1.00	69.99
15	905	N	VAL	115	31.343	-2.844	-5.309	1.00	69.99
	906	CA	VAL	115	30.680	-1.966	-4.556	1.00	39.79
	907	CB	VAL	115	29.938	-0.865	-5.530	1.00	39.79
	908	CG1	VAL	115	29.177	0.018	-3.555	1.00	39.79
	909		VAL	115	28.996	-1.485	-6.198	1.00	69.99
20	910	CG2	VAL	115	31.764	-1.376		1.00	69.99
	911	C	VAL	115	32.797	-0.930	-5.701	1.00	52.13
	912	0	TYR	116	31.540	-1.392	-7.511	1.00	52.13
	913	N	TYR	116	32.524	-0.869	-8.457		78.35
	914	CA	TYR	116		-1.988	-9.377	1.00 1.00	78.35
25	915	CB	TYR	116		-3.109	-8.650		78.35
	916	CG		116		-4.214	-8.178	1.00	78.35
	917	CD1	TYR	116		-5.247	-7.492	1.00	78.35 78.35
	918	CE1	TYR	116		-3.057	-8.419	1.00	78.35 78.35
	919	CD2	TYR	116			-7.736	1.00	78.35
30	920	CE2	TYR	116			-7.275	1.00	78.35 78.35
-	921	CZ	TYR	116		-6.180	-6.600	1.00	76.33 52.13
	922	OH	TYR	110			-9.292	1.00	
	923	С	TYR		44		-9.242	1.00	52.13
	924	0	TYR	110			-10.063	1.00	52.62
35		N	LYS	11			-10.901	1.00	52.62
55	926	CA	LYS	11			-12.102	1.00	75.37
	927	СВ	LYS	11			-13.200		75.37
	928	CG	LYS	11			-14.444	1.00	75.37
	929	CD	LYS	11			-14.904	1.00	75.37
40		CE	LYS	11			-16.222	1.00	75.37
70	931	NZ	LYS	11			-10.09	5 1.00	52.62
	932	C	LYS	11			-10.585		52.62
	933	Ō	LYS	1	17 30.41		-8.85		53.28
	934	N	VAL		18 31.85		-8.02		53.28
4:		CA	VAL		18 31.05		-6.56		39.37
٦.	936	СВ	VAL		18 31.5		-5.79	3 1.00	39.37
	937	CG1	VAL		18 30.8		-5.90		39.37
	938	CG2	VAL		18 31.2		-8.51		53.28
	939	C	VAL		18 31.0	- 400	-8.77		53.28
5	0 940	ŏ	VAL		18 32.1				50.90
J	941	Ň	ILE		119 29.8				50.90
	942	ĞA.	ILE		119 29.7			_	47.00
	942	ČВ	ILE	•	119 29.0				47.00
		ÇG2		•	119 28.8				47.00
	944	CG1			119 30.0				47.00
	55 945	CD1			119 29.				50.90
	946		ILE		119 28.7		_		50.90
	947	C	ILE		119 27.				46.78
	948	0	TYR		120 29.	087 9.429			46.78
	949	N	TYR			<u>228</u> 10.177	2 -6.7		
	60 950	CA	TYR		120 29.	018 10.75			4-74
	951	CB				508 9.72			4
	952	CG				764 9.15			
	953	CD				225 8.21	0 -3.6	342 1.00	71
	954	CE	ווו ו	•					

		000	TYR	120 ·	28.716	9.332	•	1.00	47.71
1	955	CD2 CE2	TYR	120	29.167	8.376		1.00 1.00	47.71 47.71
	956	CZ	TYR	120	30.427	7.820		1.00	47.71
	957	OH	TYR	120	30.894	6.859	-1.911 -7.483	1.00	46.78
	958	C	TYR	120	27.559	11.319	-7.463 -8.330	1.00	46.78
3	959 960	ŏ	TYR	120	28.166	11.972	-7.152	1.00	39.53
	961	Ň	TYR	121	26.306	11.572	-7.807	1.00	39.53
	962	CA	TYR	121	25.578	12.651 12.092	-8.584	1.00	51.28
	963	CB	TYR	121	24.378	11.242	-9.758	1.00	51.28
10	964	CG	TYR	121	24.767	9.897	-9.598	1.00	51.28
10	965	CD1	TYR	121	25.075 25.525	9.131	-10.673	1.00	51.28
	966	CE1	TYR	121	25.525 24.909	11.802	-11.025	1.00	51.28
	967	CD2	TYR	121 121	24. 3 03 25. 35 9	11.046	-12.106	1.00	51.28
	968	CE2	TYR	121	25.669	9.712	-11.920	1.00	51.28
15	969	CZ	TYR	121	26.158	8.978	-12.979	1.00	51.28
	970	OH	TYR TYR	121	25.079	13.703	-6.834	1.00	39.53
	971	C	TYR	121	24.692	13.392	-5.711	1.00	39.53 48.43
	972	0 N	LYS	122	25.104	14.955	-7.263	1.00	48.43
00	973	CA	LYS	122	24.584	16.022	-6.422	1.00 1.00	57.69
20	974	CB	LYS	122	25.704	16.886	-5.851 -4.630	1.00	57.69
	975 976	CG	LYS	122	25. 21 5	17.619	-4.830 -4.345	1.00	57.69
	976 977	CD	LYS	122	25.990	18.882	-4.345 -5.251	1.00	57.69
	978	CE	LYS	122	25.543	19.987 21.258	-4.865	1.00	57.69
25	979	NZ	LYS	122	26.178	16.871	-7.296	1.00	48.43
LJ	980	C	LYS	122	23.658	17.523	-8.231	1.00	48.43
	981	0	LYS	122	24.108 22.368	16.861	-6.983	1.00	47.40
	982	N	ASP	123	21.384	17.609	·-7.783	1.00	47.40
	983	CA	ASP	123 123	21.625	19.122	-7.687	1.00	49.57
30	984	CB	ASP	123	21.713	19.611	-6.269	1.00	49.57
	985	CG	ASP ASP	123	20.803	19.311	-5.468	1.00	49.57
	986	OD1	ASP	123	22.699	20.301	-5.953	1.00	49.57 47.40
	987	OD2 C	ASP	123		17.197	-9.241	1.00 1.00	47.40
25	988	Ö	ASP	123	21.856	18.044	-10.095	1.00	52.66
35	989	N	GLY	124	21.433	15.904	-9.521 -10.888	1.00	52.66
	990 991	CA	GLY	124		15.430	-11.421	1.00	52.66
	992	Ċ.	GLY	124		15.363	-12.041	1.00	52.66
	993	Ö	GLY	124		14.382 16.408	-11.204	1.00	53.89
40		N	GLU	125	23.807	16.447	-11.672	1.00	53.89
	995	CA	GLU	125		17.841	-11.427	1.00	115.76
	996	CB	GLU	129		18.952	-12.208	1.00	115.76
	997	CG	GLU	12: 12:		18.876	-13.689	1.00	115.76
	998	CD	GLU	12		18.910	-14.044		115.76
45		OE1	GLU	72	-	18.784	-14.498		115.76 53.89
	1000	OE2 C	GLU	12	5 26.085	15.412	-10.974		53.89
	1001 1002	ŏ	GLU	12	5 25.912	15.130	-9. 79 0 -11. 70 9		51.23
	1002	Ň	ALA	12		14.847	-11.709		51.23
5		CA	ALA	12		13.880 12. 99 6	-12.218		49.62
,	1005	CB	ALA	12		14.673	-10.422		51.23
	1006	С	ALA	12		15.551	-11.020		51.23
	1007	0	ALA		26 29.659 27 29.302	14.373	-9.15		63.08
	1008	N	LEU		27 29.302 27 30.332	15.088	-8.40		63.08
5	5 1009	CA	LEU		27 30.641	14.370	-7.10		50.82
	1010	CB	LEU		27 29.663	14.719	-6.00		50.82
	1011	CG	LEU		27 30.265	14.281	-4.68		50.82 50.82
	1012	CD1 CD2			27 29.403	16.221	-6.00		63.08
	1013	CDZ	LEU		27 31.643	15.322	-9.14		63.08
•	50 1014 1015	ő	LEU		27 32.233		-9.68		120.62
	1016	Ň	LYS	1	28 32.096		-9.13 -9.78		120.62
	1017	CA	LYS		28 33.343		-9.76 -10.12		105.58
	1018	ÇB	LYS	1	128 33.360	18.423	- 10.12		

	1019 1020 1021	CG CD CE	LYS LYS LYS	128 128	32.187 32.494 31.295 30.167	18.879 20.181 20.661 21.011	-10.946 -11.667 -12.465 -11.563	1.00 1.00 1.00	105.58 105.58 105.58 105.58
5	1022 1023 1024	NZ C O	LYS LYS LYS	128 128 128	34.535 35.604	16.589 16.232 16.714	-8.883 -9.381 -7.568	1.00 1.00 1.00	120.62 120.62 102.50
	1025 1026	N CA CB	TYR TYR TYR	129 129 129	34.353 35.415 34.823	16.387 16.167	-6.613 -5.216 -4.528	1.00 1.00 1.00	102.50 91.38 91.38
10	1027 1028 1029	CG CD1	TYR TYR TYR	129 129 129	34.316 32.980 32.519	17.406 17.523 18.664	-4.148 -3.477	1.00 1.00	91.38 91.38 91.38
	1030 1031 1032	CE1 CD2 CE2	TYR TYR TYR	129 129 129	35.187 34.741 33.408	18.455 19.598 19.699	-4.224 -3.557 -3.185	1.00 1.00 1.00	91.38 91.38
15	1033 1034 1035	CZ OH C	TYR TYR	129 129 129	32.960 36.133 35.553	20.831 15.099 14.244	-2.533 -7.024 -7.692	1.00 1.00 1.00	91.38 102.50 102.50
20	1036 1037 1038	O N CA	TYR TRP TRP	130 130	37.394 38.102 39.605	14.948 13.709 13.916	-6.636 -6.940 -7.127	1.00 1.00 1.00	95.53 95.53 77.30
	1039 1040 1041	CB CG CD2	TRP TRP TRP	130 130 130	40.317 40.414	12.599 11.594 10.447	-7.015 -8.027 -7.440	1.00 1.00 1.00	77.30 77.30 77.30
25	1042 1043 1044	CE2 CE3 CD1	TRP TRP TRP	130 130 130	41.001 40.046 40.853	11.536 12.046 10.752	-9.379 -5.881 -6.124	1.00 1.00 1.00	77.30 77.30 77.30
	1045 1046 1047	NE1 CZ2 CZ3	TRP TRP TRP	130 130 130	41.262 41.229 40.278	9.269 10.365	-8.149 -10.083 -9.469	1.00 1.00 1.00	77.30 77.30 77.30
30	1048 1049 1050	CH2 C O	TRP TRP TRP	130 130 130	40.862 37.903 38.038	9.250 12.742 13.124	-5.784 -4.620 -6.091	1.00 1.00 1.00	95.53 95.53 71.08
25	1051 1052	N CA CB	TYR TYR TYR	131 131 131	37.589 37.397 35.934	11.488 10.505 10.495	-5.034 -4.565 -5.657	1.00 1.00 1.00	71.08 66.47 66.47
35	1053 1054 1055	CG CD1 CE1	TYR TYR TYR	131 131 131	34.370	10.405 9.178 9.111	-6.055 -7.009	1.00 1.00 1.00	66.47 66.47 66.47
40	1056 1057 1058 1059	CD2 CE2 CZ	TYR TYR TYR	131 131 131	33.375 32.857	11.562 11.506 10.283	-6,246 -7,201 -7,572 -8,477	1.00 1.00 1.00	66.47 66.47 66.47
	1060 1061 1062	OH C O	TYR TYR TYR	13 ¹ 13 ¹ 13	37.838 38.058	10.246 9.098 8.768	-5.384 -6.554 -4.345	1.00 1.00	71.08 71.08 130.21
45	1063 1064 1065	N CA CB	GLU GLU	13: 13: 13:	2 38.389 2 39.252	8.277 6.884 6.520	-4.467 -3.266 -1.959	1.00 1.00	130.21 141.76 141.76
50	1066 1067	CG CD OE1	GLU GLU	13 13 13	2 39.311 2 40.544	6.649 7.221 7.379	-0.824 -0.985 0.235	1.00	141.76 141.76 141.76
)(1069 1070 1071	OE2 C O	GLU GLU GLU	13 13 13	37.135 32 36.031	6.503	-4.479 -4.23 -4.74	1.00 4 1.00	130.21 130.21 122.18
5	1072 5 1073 1074	N CA CB	ASN ASN ASN	13	33 36.182 33 36.698	3.803 2.392	-4.79 -5.09 -5.50	4 1.00 0 1.00	122.18 141.76 141.76
	1075 1076 1077	CG OD1 ND2	ASN ASN	1:	33 35.592 33 34.412 33 35.980	1.777	-5.52 -5.83 -3.50	2 1.00 1 1.00	141.76 141.76
ϵ	50 1078 1079	C O N	ASN ASN HIS	1	33 35.348 33 35.879 34 34.044	3.627 4.032	-2.40 -3.68	6 1.00 31 1.00	122.18 110.94
	1080 1081 1082	CA CB	HIS HIS	1	34 33.010 34 32.500		-2.63 -2.35		

	1083	CG	HIS	134 ·	33.300	1.858	-1.341	1.00	116.53
	1084	CD2	HIS	134	33.153	1.742	-0.001	1.00	116.53
	1085	ND1	HIS		34.341	1.029	-1.687	1.00	116.53
	1086	CE1	HIS	134	34.797	0.425	-0.605	1.00	116.53
5	1087	NE2	HIS	134	34.091	0.837	0.431	1.00	116.53
,	1088	C	HIS	134	33.169	4.773	-1.283	1.00	110.94
	1089	ŏ	HIS	134	32.312	4.627	-0.408	1.00	110.94
	1009	Ň	ASN	135	34.245	5.532	-1.105	1.00	107.95
		CA	ASN	135	34.430	6.296	0.125	1.00	107.95
10	1091	CB	ASN	135	35.464	5.654	1.057	1.00	141.21
10	1092	CG	ASN	135	35.389	6.207	2.490	1.00	141.21
	1093	OD1	ASN	135	34.538	7.044	2.801	1.00	141.21
	1094	ND2	ASN	135	36.271	5.735	3.358	1.00	141.21
	1095		ASN	135	34.900	7.680	-0.310	1.00	107.95
15	1096	C O	ASN	135	35.952	7.836	-0.925	1.00	107.95
15	1097	N	ILE	136	34.095	8.685	-0.005	1.00	65.75
	1098	CA	ILE	136	34.421	10.048	-0.387	1.00	65.75
	1099		ILE	136	33.401	10.550	-1.433	1.00	65.18
	1100	CB CG2	ILE	136	32.002	.3.306	-0.943	1.00	65.18
20	1101	CG2	ILE	136	33.587	12.030	-1.717	1.00	65.18
20	1102	CD1	ILE	136	32.601	12.535	-2.780	1.00	65.18
	1103		ILE	136	34.457	10.983	0.826	1.00	65.75
	1104	C	ILE	136	33.593	10.924	1.706	1.00	65.75
	1105	0	SER	137	35.475	11.838	0.863	1.00	51.67
0.5	1106	N		137	35.646	12.785	1.957	1.00	51.67
25	1107	CA	SER	137	36.944	12.470	2.714	1.00	87.54
	1108	CB	SER	137	37.068	13.249	3.889	1.00	87.54
	1109	og	SER	137	35.678	14.225	1.449	1.00	51.67
	1110	C	SER	137	36.522	14.593	0.629	1.00	51.67
20	1111	0	SER	138	34.729	15.021	1.924	1.00	63.18
30	1112	N	ILE	138	34.634	16.431	1.559	1.00	63.18
	1113	CA	ILE	138	33.178	16.801	1.239	1.00	64.58
	1114	CB	ILE	138	33.030	18.301	1.103	1.00	64.58
	1115	CG2	ILE	138	32.754	16.080	-0.043	1.00	64.58
25	1116	CG1	ILE	138	31.285	16.134	-0.328	1.00	64.58
35	1117	CD1	ILE	138	35.119	17.126	2.815	1.00	63.18
	1118	C	ILE ILE	138	34.379	17.271	3.786	1.00	63.18
	1119	0		139	36.384	17.525	2.783	1.00	80.92
	1120	N	THR	139	37.063	18.140	3.920	1.00	80.92
40	1121	CA	THR	139	38.557	18.282	3.609	1.00	76.51
40	1122	CB	THR	139	38.721	19.040	2.403	1.00	76.51
	1123	OG1	THR	139	39.189	16.909	3.432	1.00	76.51
	1124	CG2	THR THR	139	36.576	19.468	4.498	1.00	80.92
	1125	C	THR	139	36.484	19.612	5.721	1.00	80.92
45	1126	0	ASN	140	36.277	20.441	3.644	1.00	57.80
45	1127	N	ASN	140	35.837	21.738	4.151	1.00	57.80
	1128	CA	ASN	140	36.840	22.821	3.731	1.00	95.08
	1129	CB CG	ASN	140	37.066	23.863	4.812	1.00	95.08
	1130	OD1	ASN	140	36.122	24.315	5.458	1.00	95.08
50	1131	ND2	ASN	140	38.320	24.259	5.005	1.00	95.08
20			ASN	140	34.438	22.108	3.657	1.00	57.80
	1133	C O	ASN	140	34.300	22.924	2.752	1.00	57.80
	1134		ALA	141	33.413	21.512	4.265	1.00	63.45
	1135	N	ALA	141	32.031	21.765	3.871	1.00	63.45
55	1136	CA CB	ALA	141	31.060	21.206	4.914	1.00	40.09
55				141	31.740	23.242	3.642	1,00	63.45
	1138	CO	ALA ALA	141	32.185	24.106	4.399	1.00	63.45
	1139			142	30.971	23.505	2.588	1.00	60.40
	1140	N	THR	142	30.573	24.847	2.192	1.00	60.40
40	1141	CA	THR THR	142	31.247	25.210	0.871	1.00	65.36
60	1142	CB OG1	THR	142	32.580	25.646	1.137	1.00	65.36
	1143	CG2	THR	142	30.489	26.292	0.144	1.00	65.36
	1144		THR	142		24.871	2.017	1.00	60.40
	1145 1146	C O	THR	142		23.815	1.955	1.00	60.40
	1140	U	IDD	172	20.402				

				143 .	28.471	26.061			51.83
	1147	• •	VAL	143	27.031	26.150		1.00	51.83
	1148	CA	VAL	143	26.547	27.626		1.00	51.35
	1149	CB	VAL VAL	143	27.058	28.335	0.507	1.00	51.35
_	1150	CG1	VAL	143	25.019	27.673	1.807	1.00	51.35
5	1151	CG2	VAL	143	26.667	25.448	0.434	1.00	51.83
	1152	C	VAL	143	25.584	24.884	0.292	1.00	51.83 54.88
	1153	O N	GLU	144	27.599	25.466	-0.513	1.00	54.88
	1154	CA	GLU	144	27.411	24.836	-1.812	1.00 1.00	66.83
10	1155	CB	GLU	144	28.554	25.200	-2.749	1.00	66.83
10	1156	CG	GLU	144	28.639	26.639	-3.146	1.00	66.83
	1157	CD	GLU	144	29.941	26.929	-3.860 -4.799	1.00	66.83
	1158 1159	OE1	GLU	144	30.280	26.169	-4.7 99 -3.478	1.00	66.83
	1160	OE2	GLU	144	30.624	27.908	-1.754	1.00	54.88
15	1161	C	GLU	144	27.348	23.308	-2.685	1.00	54.88
13	1162	ŏ	GLU	144	26.862	22.675 22.707	-0.692	1.00	47.71
	1163	Ň	ASP	145	27.869	21.258	-0.607	1.00	47.71
	1164	CA	ASP	145	27.840	20.746	0.360	1.00	46.72
	1165	СВ	ASP	145	28.902	21.045	-0.116	1.00	46.72
20	1166	CG	ASP	145	30.292	20.700	-1.268	1.00	46.72
20	1167	OD1	ASP	145	30.613	21.629	0.667	1.00	46.72
•	1168	OD2	ASP	145	31.077	20.785	-0.200	1.00	47.71
	1169	С	ASP	145	26.463 26.227	19.592	-0.055	1.00	47.71
	1170	0	ASP	145	25.549	21.727	-0.007	1.00	42.81
25	1171	N	SER	146	25.54 5 24.175	21.355	0.314	1.00	42.81
	1172	CA	SER	146 146	23.363	22.573	0.750	1.00	49.76
	1173	CB	SER	146	23.841	23.139	1.955	1.00	49.76
	1174	QG	SER	146	23.583	20.794	-0.993	1.00	42.81
	1175	C	SER	146	24.014	21.160	-2.091	1.00	42.81
30	1176	0	SER GLY	147	22.611	19.905	-0.879	1.00	56.97
	1177	N	GLY	147		19.334	-2.064	1.00	56.97 56.97
	1178	CA	GLY	147		17. 9 75	-1.766	1.00	56.97
	1179	C	GLY	147	21.382	17.546	-0.612	1.00 1.00	35.67
٥.	1180	N	THR	148		17.294	-2.797	1.00	35.67
35		CA	THR	148		15.968	-2.594	1.00	41.21
	1182	CB	THR	148		15.784	-3.251 -4.522	1.00	41.21
	1183	OG1	THR	148		15.127		1.00	41.21
	1184 1185	CG2	THR	148	18.251	17.118	-3.427 -3.297	1.00	35.67
40	1186	č	THR	148		15.106	-4.382	1.00	35.67
40	1187	Ö	THR	148		15.447 13.998	-2.668	1.00	37.71
	1188	N	TYR	149			-3.233	1.00	37.71
	1189	CA	TYR	149		13.118 13.045	-2.317	1.00	40.71
	1190	CB	TYR	14		14.300	-2.117	1.00	40.71
4:		CG	TYR	14		15.396	-1.442	1.00	40.71
•	1192	CD1	TYR	14		16.544	-1.214	1.00	40.71
	1193	CE1	TYR	14		14.366	-2.568	1.00	4G.71
	11 94	CD2	TYR	14 14		15,494	-2.357	1.00	40.71
	1195	CE2	TYR	14		16.581	-1.680		40.71
5	0 1196	CZ	TYR TYR	14		17.712	-1.506		40.71
	1197	OH	TYR	14		11.701	-3.349		37.71
	1198	C	TYR		9 21.256	11.316	-2.690		37.71 32.88
	1199	0	TYR		50 22.918	10.930	-4.183		32.88
	1200	N CA	TYR		50 22.629	9.526	-4.33		48.85
	5 1201	CB	TYR		50 21.325	9.288	-5.12		48.85
	1202	CG	TYR		50 21.384	9.537	-6.60		48.85
	1203 1204	CD1	TYR	1	50 21.813		-7.48		48.85
	1204	CE1	TYR		50 21.854		-8.85	_	48.85
	60 1206	CD2	TYR		50 20.997		-7.13 -8.50		48.85
,	1207	CE2	TYR		50 21.038		-8.50 -9.35		48.85
	1208	CZ	TYR		50 21.470		-9.35 -10.70		48.85
	1209	OH	TYR		50 21.566		-5.04		32.88
	1210	C	TYR	1	150 23.853	9.009	-5.0		

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					4 000	9.802	-5.513	1.00	32.88
	1211	0	TYR		4.668	7.699	-5.108	1.00	43.72
	1212	N	CYS		24.018 25.173	7.055 7.151	-5.793	1.00	43.72
	1213	CA	CYS		25.173 24.734	5.984	-6.660	1.00	43.72
	1214	C .	CYS			5.457	-6.488	1.00	43.72
5	1215	0	CYS		23. 63 4 26. 22 9	6.672	-4,779	1.00	45.51
•	1216	CB	CYS		25.716	5.340	-3.631	1.00	45.51
	1217	SG	CYS		25.710 25.605	5.601	-7.588	1.00	49.22
	1218	N	THR		25.366	4.470	-8.467	1.00	49.22
	1219	CA	THR		25.033	4.892	-9.940	1.00	42.84
10	1220	CB	THR		26.153	5.566	-10.535	1.00	42.84
	1221	OG1	THR		23.823	5.794	-9.968	1.00	42.84
	1222	CG2	THR		26.647	3.655	-8.467	1.00	49.22
	1223	Ç	THR		27.752	4.192	-8,290	1.00	49.22
	1224	0	THR	153	26.501	2.352	-8.638	1.00	49.54
15	1225	N	GLY	153	27.664	1.499	-8.669	1.00	49.54
	1226	CA	GLY	153	27.298	0.134	-9.203	1.00	49.54
	1227	C	GLY	153	26.118	-0.243	-9.243	1.00	49.54
	1228	0	GLY	154	28.314	-0.610	-9.618	1.00	50.10
	1229	N	LYS LYS	154	28.108	-1.946	-10.141	1.00	50.10
20	1230	CA	LYS	154	29.078	-2.209	-11.297	1.00	64.36
	1231	CB	LYS	154	28.956	-3.599	-11.885	1.00	64.36
	1232	CG	LYS	154	30.078	-3.925	-12.851	1.00	64.36
	1233	CD	LYS	154	30.006	-5.382	-13.286	1.00	64.36
	1234	CE	LYS	154	31.019	-5.728	-14.324	1.00	64.36
25	1235	NZ	LYS	154	28.310	-2.994	-9.048	1.00	50.10
	1236	C	LYS	154	29.402	-3.123	-8.497	1.00	50.10 62.56
	1237	N	VAL	155	27.236	-3.709	-8.714	1.00	62.56
	1238	CA	VAL	155	27.295	-4.784	-7.727	1.00 1.00	41.01
20	1239	CB	VAL	155	26.139	-4.722	-6.732	1.00	41.01
30	1240 1241	CG1	VAL	155	26.266	-5.872	-5.742 -6.009	1:00	41.01
	1242	CG2	VAL	155	26.132	-3.391	-8.546	1.00	62.56
	1243	Č	VAL	155	27.163	-6.063	-9.312	1.00	62.56
	1244	Ö	VAL	155	26.211	-6.224 6.075	-8.380	1.00	74.40
35	1245	N	TRP	156	28.110	-6.975 -8.205	-9,159	1.00	74.40
33	1246	CA	TRP	156	28.104	-9.049	-8.887	1.00	64.29
	1247	CB	TRP	156	26.846	-9.536	-7.464	1.00	64.29
	1248	CG	TRP	156	26.728	-10.497	-6.808	1.00	64.29
	1249	CD2	TRP	156	27.569 27.114	-10.605	-5.472	1.00	64.29
40		CE2	TRP	156	28.661	-11.276	-7.218	1.00	64.29
	1251	CE3	TRP	156	25.826	-9.119	-6.528	1.00	64.29
	1252	CD1	TRP	156	26.052	-9.753	-5.330		64.29
	1253	NE1	TRP	156 156	27.717	-11.464	-4.537	1.00	64.29
	1254	CZ2	TRP	156	29.260	-12.130	-6.290		64.29
45		CZ3	TRP TRP	156	28.783	-12.215	-4.961		64.29
	1256	CH2	TRP	156	28.162	-7.814	-10.639		74.40
	1257	C	TRP	156	29.121	-7.178	-11.088		74.40
	1258	0	GLN	157	27.128	-8.163	-11.397		71.89
	1259	N CA	GLN	157	27.132	-7.841	-12.823		71.89 111.42
50		CB	GLN	157		-9.105	-13.650		111.42
	1261	CG	GLN	157		-10.072	-13.672		111.42
	1262	CD	GLN	157	29.351	-9.380	-13.965		111.42
	1263 1264	OE1	GLN	157	29.504	-8.683	-14.969		111.42
5		NE2	GLN	157		-9.570	-13.08		71.89
ر	1266	C	GLN	157		-6.731	-13.292 -14.47		71.89
	1267	ŏ	GLN	157		-6.418			61.40
	1268	Ň	LEU	158		-6.124	-12.38		61.40
	1269	ĊA	LEU	158		-5.0 6 1	-12.78 -12.46		60.41
4	60 1270	CB ·	LEU	158		-5.463	-12.40 -13.11		60.41
	1271	CG	LEU	158		-6.756 6.049	-13.11 -12.77		60.41
	1272	CD1	LEU	15		-6.948 6.677	-14.60		60.41
	1273	CD2	LEU	15		-6.677 -3.703	-12.14		61.40
	1274	С	LEU	15	8 24.822	-3.103	- 1 1		

	1275	O N	LEU ASP	159	25.619 24.167	-3.596 -2.668	-11.213 -12.662 -12.140	1.00 1.00 1.00	61.40 56.42 56.42
	1276 1277	CA .	ASP	159	24. 338 24. 46 5	-1.322 -0.311	-13.276	1.00	74.24
	1278	CB	ASP	159 159	25.653	-0.586	-14.170	1.00	74.24
	1279	CG OD1	ASP ASP	159	26.794	-0.666	-13.663	1.00 1.00	74.24 74.24
	1280	OD2	ASP	159	25.444	-0.721	-15.392 -11.282	1.00	56.42
	1281 1282	C	ASP	159	23.135	-6.972 -1.211	-11.680	1.00	56.42
	1283	0	ASP	159 160	21.992 23.390	-0.419	-10.098	1.00	43.45
10	1284	N	TYR TYR	160	22.303	-0.038	-9.214	1.00	43.45 50.12
	1285	CA CB	TYR	160	22.309	-0.884	-7.936 -8.182	1.00 1.00	50.12
	1286 1287	CG	TYR	160	22.158	-2.369 -3.115	-8.705	1.00	50.12
	1288	CD1	TYR	160	23.210 23.076	-4.483	-8.933	1.00	50.12
15	1289	CE1	TYR TYR	160 160	20.961	-3.026	-7.896	1.00	50.12 50.12
	1290	CD2 CE2	TYR	160	20.814	-4.392	-8.121 -8.637	1.00 1.00	50.12
	1291 1292	CZ	TYR	160	21.875	-5.113 6.467	-8.840	1.00	50.12
	1293	OH	TYR	160	21.760 22.384	-6.467 1.437	-8.868	1.00	43.45
20	1294	C	TYR	160 160	23.341	2.125	-9.219	1.00	43.45
	1295	0	TYR GLU	161	21.370	1.922	-8.175	1.00 1.00	46.75 46.75
	1296 1297	N CA	GLU	161	21.304	3.318	-7.810 -8.847	1.00	65.60
	1298	CB	GLU	161	20.454	4.057 5.421	-8.439	1.00	65.60
25	1299	CG	GLU	161 161	19.930 19.318	6.190	-9.614	1.00	65.60
	1300	CD	GLU GLU	161	18.653	7.226	-9.377	1.00 1.00	65.60 65.60
	1301 1302	OE1 OE2	GLU	161	19.517	5.765	-10.777 -6.432	1.00	46.75
	1302	C	GLU	161	20.687	3.385 2.702	-6.148	1.00	46.75
30	1304	0	GLU	161		4.190	-5.559	1.00	41.55
	1305	N	SER SER	162 162		4.297	-4.202	1.00	41.55 41.77
	1306	CA CB	SER	162	21.841	4.761	-3.241 -3.467	1.00 1.00	41.77
	1307 1308	OG	SER	162		6.124 5.311	-4.170	1.00	41.55
35	1309	C	SER	162		6.079	-5.103	1.00	41.55
-	1310	0	SER GLU	162 163		5.294	-3.088	1.00	45.18 45.18
	1311	N CA	GLU	163	3 17.794	6.261	-2.881 -1.632	1.00 1.00	80.94
	1312 1313	CB	GLU	163		5.907 4.687	-1.787		80.94
40		CG	GLU	16 16		4.941	-2.730	1.00	80.94
	1315	CD	GLU GLU	16		5.812	-2.407	1.00	80.94 80.94
	1316	OE1 OE2	GLU	16	3 14.922	4.285	-3.794 -2.653		45.18
	1317 1318	C	GLU	16		7.576 7.581	-2.236		45.18
45	1319	0	GLU	16 16		8.709	-2.92	1.00	47.28
	1320	N	PRO PRO	16		8.936	-3.57		31.71 47.28
	1321	CD CA	PRO	16	34 18.598	9.970	-2.71: -3.67	2 1.00 7 1.00	31.71
	1322 1323	CB	PRO		64 17.888	10.913 10.450	-3.55		31.71
5	0 1324	CG	PRO		64 16.472 64 18.525	10.444	-1.25	6 1.00	47.28
	1325	Ç	PRO PRO		64 17.624	10.084	-0.49		47.28 31.92
	1326 1327	0 N	LEU		65 19.480	11.263	-0.86 0.49		31.92
	1328	CA	LEU		65 19.513		1.22		52.60
5	5 1329	СВ	LEU		65 20.705 65 21.098		2.56	1.00	52.60
_	1330	CG	LEU		65 21.098 65 19.980		3.56		52.60 50.60
	1331	CD1 CD2			65 22.404	11.139	3.02		52.60 31.92
	1332 1333	CDZ	LEU	1	165 19.697	13.275	0.44 -0.4		
- 1	50 1334	ŏ	LEU		165 20.401		1.3		38.25
`	1335	N	ASN		166 19.084 166 19.297		1.3	45 1.00	38.25
	1336		ASN ASN		166 17.969	16.186	1.5		
	1337 1338		ASN		166 17.056		0.3	09 1.00	, 30.13
	1330								

Į.

	1339 1340 1341 1342	OD1 ND2 C	ASN ASN ASN ASN	166 166 166	17.546 15.748 20.341 20.282	15.847 16.259 15.889 15.480	0.490 2.398 3.561	1.00 1.00 1.00 1.00 1.00	38.79 38.79 38.25 38.25 41.84
5	1343 1344 1345	N CA CB CG2	ILE ILE ILE ILE	167 167 167 167	21.309 22.326 23.732 24.814	16.695 17.187 16.672 17.546	2.894 2.516	1.00 1.00 1.00 1.00	41.84 52.89 52.89 52.89
10	1346 1347 1348 1349	CG1 CD1 C	ILE ILE ILE ILE	167 167 167 167	23.884 25.008 22.356 22.535	15.227 14.493 18.698 19.347	2.326 2.934 1.905	1.00 1.00 1.00 1.00	52.89 41.84 41.84 49.92
15	1350 1351 1352 1353 1354	N CA CB OG1	THR THR THR THR	168 168 168 168	22.194 22.213 20.999 19.818	19.250 20.694 21.151 20.706 22.658	4.132 4.336 5.122 4.465 5.238	1.00 1.00 1.00 1.00	49.92 52.27 52.27 52.27
20	1355 1356 1357 1358	CG2 C O N	THR THR THR VAL	168 168 168 169	20.977 23.434 23.768 24.078	21.157 20.577 22.216	5.126 6.156 4.649 5.331	1.00 1.00 1.00 1.00	49.92 49.92 52.96 52.96
20	1359 1360 1361 1362	CA CB CG1 CG2	VAL VAL VAL	169 169 169 169	25.230 26.359 27.578 26.710	22.791 23.106 23.646 21.865	4.346 5.112 3.560 6.037	1.00 1.00 1.00 1.00	44.29 44.29 44.29 52.96
25	1363 1364 1365	C O N CA	VAL VAL ILE ILE	169 169 170 170	24.837 24.456 24.920 24.585	24.102 25.058 24.138 25.345	5.373 7.372 8.146 9.380	1.00 1.00 1.00 1.00	52.96 52.65 52.65 54.27
30	1366 1367 1368 1369 1370	CB CG2 CG1 CD1	ILE ILE ILE ILE	170 170 170 170	23.700 22.411 24.473 23.644	25.033 24.342 24.181 23.798	8.945 10.390 11.619 8.638	1.00 1.00 1.00 1.00	54.27 54.27 54.27 52.65
35	1371 1372 1373	C O N CA	ILE ILE LYS LYS	170 170 171 171	25.841 26.931 25.697 26.849	26.060 25.488 27.308 28.070	8.620 9.075 9.551 9.470	1.00 1.00 1.00 1.00	52.65 92.13 92.13 112.78
40	1374 1375 1376 1377 1378	CB CG CD CE	LYS LYS LYS LYS	171 171 171 171 171		29.574 30.436 31.881 32.008 33.430	9.745 9.293 7.772 7.310	1.00 1.00 1.00 1.00	112.78 112.78 112.78 112.78
	1379 1380 1381 1382	NZ C O N	LYS LYS LYS ALA	171 171 172 172	27.244 26.388 28.551	27.674 27.384 27.662 27.282	10.974 11.812 11.230 12.529	1.00 1.00 1.00 1.00	92.13 92.13 124.64 124.64
45	1384 1385 1386	CA CB C	ALA ALA ALA ALA	172 172 173 173	30.617 2 28.457 2 28.071	27.553 27.910 27.191 29.254	12.537 13.772 14.695 13.819	1.00 1.00 1.00 1.00	104.18 124.64 124.64 141.76
50	1389 1390	N CD CA CB	PRO PRO PRO PRO	17: 17: 17: 17: 17:	3 28.819 3 27.730 3 27.492	30.230 29.953	12.825 14.963 14.415 13.575	1.00 1.00	113.27 141.76 113.27 113.27
5	1391 1392 5 1393 1394	CG C O N	PRO PRO PRO ARG	17 17 17	23 26.461 23 25.733	29.332 28.603 29.644	15.553 14.876 16.826 17.592	1.00 1.00 2 1.00	141.76 141.76 135.93 135.93
(1395 1396 1397 50 1398	CA CB CG CD	ARG ARG ARG ARG ARG	17 17 1	74 24.358 74 25.304 74 24.573 74 25.519	30.340 31.216 32.197	19. 9 69 20.75	5 1.00 5 1.00 5 1.00	141.76 141.76 141.76 141.76
	1399 1400 1401 1402	NE CZ NH1 NH2	ARG ARG	1	74 25.178 74 23.90 74 26.11	33.813 33.970	21.74 22.07 22.40	1 1.00	141.76 141.76 141.76

							40 706	1.00	135.93
	4.400	С	ARG	174 .	24.068	28.322	16.796 16.923		135.93
	1403 1404	ŏ	ARG	174	24.026	27.095	14.864		113.42
	1404	C1	NAG	21A	25.553	-8.090 -8.923	13.694		113.42
	1406	C2	NAG	21A	26.103	-8.533	12.455	1.00	113.42
5	1407	N2	NAG	21A	25.455 26.186	-8.153	11.409	1.00	113.42
,	1408	C7	NAG	21A	27.417	-8.115	11.428	1.00	113.42
	1409	07	NAG	21A 21A	25.43fi	-7.756	10.148	1.00	113.42
	1410	C8	NAG NAG	21A	25.876	-10.419	13.955	1.00	113.42 113.42
	1411	C3	NAG	21A	26.513	-11.185	12.940	1.00 1.00	113.42
10	1412	O3 C4	NAG	21A	26.441	-10.817	15.323 15.616	1.00	113.42
	1413	04	NAG	21A	26.084	-12.164	16.423	1.00	113.42
	1414 1415	C5	NAG	21A	25.905	-9.887 -8.502	16.092	1.00	113.42
	1416	O5	NAG	21A	26.175	-10.164	17.760	1.00	113.42
15	1417	C6	NAG	21A	26.569 26.198	-9.199	18.732	1.00	113.42
••	1418	O6	NAG	21A 42A	9.440	5.012	15.315	1.00	74.70
	1419	C1	NAG NAG	42A	8.867	3.648	14.939	1.00	74.70 74.70
	1420	C2	NAG	42A	9.315	2.609	15.844	1.00	74.70 74.70
41.50	1421	N2 C7	NAG	42A	8.618	2.342	16.941	1.00 1.00	74.70
20	1422	07	NAG	42A	7.605	2.973	17.251 17.840	1.00	74.70
	1423 1424	C8	NAG	42A	9.129	1.223	13.516	1.00	74.70
	1424	C3	NAG	42A	9.294	3.312 2.058	13.131	1.00	74.70
	1426	03	NAG	42A	8.752	4.399	12.538	1.00	74.70
25	1427	C4	NAG	42A	8.835 9.4 6 9	4.168	11.266	1.00	74.70
20	1428	04	NAG	42A 42A	9.469	5.795	13.046	1.00	74.70
	1429	C5	NAG	42A	8.894	6.001	14.433	1.00	74.70
	1430	O5	NAG NAG	42A		6.900	12.259	1.00	74.70 74.70
	1431	C6 O6	NAG	42A		7.808	11.744	1.00 1.00	81.02
30	1432	C1	NAG	42B	8.771	3.603	10.203 8.945	1.00	81.02
	1433 1434	C2	NAG	42B		3.832	8.651	1.00	81.02
	1435	N2	NAG	42E		5.248 5.828	8.641	1.00	81.02
	1436	C7	NAG	42E		5.214	8.866	1.00	81.02
35	1437	07	NAG	42E 42E	3 11.980 3 10.986	7.317	8.327	1.00	81.02
•	1438	C8	NAG	42E		3.068	7.750		81.02
	1439	C3	NAG NAG	421		3.298	6.616		81.02 81.02
	1440	O3	NAG	421		1.604	8.138		81.02
40	1441	C4 O4	NAG	42	B 8.834	0.730	7.000 9.341		81.02
40) 1442 1443	C5	NAG	42		1.393	10.472		81.02
	1444	O 5	NAG	42		2.187 -0.057	9.812		81.02
	1445	C6	NAG	42		-0.235	10.916	1.00	81.02
	1446	·O6	NAG	42 42		0.362	6.612		121.66
4:	5 1447	C1	MAN	42		0.370	5.06		121.66
	1448	C2	MAN MAN	42		1.176	4.523		121.66 121.66
	1449	O2 C3	MAN		C 7.571	-1.048	4.48		121.66
	1450	03	MAN		2C 8.850	-1.599	4.75 5.04		121.66
5	1451 0 1452	C4	MAN		2C 6.480	-1.965 -1.845	4.27	_	121.66
ر	1453	04	MAN		2C 5.296	-1.621	6.51		121.66
	1454	C5	MAN		2C 6.167 2C 7.300		7.12		121.66
	1455	Q5	MAN				7.33		121.66
	1456	C6	MAN		2C 5.858 2C 5.372		6.52		121.
5	55 1457	06	MAN NAG		66A 14.879		-0.65		
	1458	C1	NAG		66A 13.401	16.282	-0.27		
	1459	C2 N2	NAG		66A 13.208		0.26 1.56		
	1460 1461	C7	NAG	1	66A 12.951		1.50 2.39		
	60 1462		NAG		66A 12.855		2.0		
	1463		NAG		166A 12.765		-1.5		69.14
	1464	. С3	NAG		166A 12.51		-1.1	47 1.00	69.14
	1465	03			166A 11.139 166A 12.83		-2.2		
	1466		NAG		1007 12.00				

				166A - 1	12 124	17.873	-3.464	1.00	69.14
	1467	04	NAG	166A	14.346	17.962	-2.463	1.00	69.14
	1468	C5	NAG	166A	15.072	17.789	-1.224	1.00	69.14
	1469	O5 .	NAG		14.736	19.321	-3.074	1.00	69.14
	1470	C6	NAG		15.449	20.162	-2.169	1.00	69.14
	1471	06	NAG NAG		11.515	19.084	-3.754	1.00	88.70 88.70
	1472	C1	NAG		11.108	19.132	-5.235	1.00	88.70
	1473	C2	NAG		12.288	19.054	-6.081	1.00	88.70
	1474	N2	NAG	166B	12.566	17.929	-6.736	1.00	88.70
	1475	C7	NAG	166B	11.857	16.927	-6.667	1.00 1.00	88.70
10	1476	O7 C8	NAG	166B	13.816	17.904	-7.601	1.00	88.70
	1477	C3	NAG	166B	10.337	20.432	-5.516 -6.848	1.00	88.70
	1478	03	NAG	166B	9.844	20.426	-6.646 -4.535	1.00	88.70
	1479	C4	NAG	166B	9.165	20.603	-4.535 -4.731	1.00	88.70
15	1480 1481	04	NAG	166B	8.572	21.908	-3.089	1.00	88.70
15	1482	C5	NAG	166B	9.688	20.469 19.203	-2.919	1.00	88.70
	1483	O5	NAG	166B	10.358		-2.021	1.00	88.70
	1484	75	NAG	166B	8.612	20.538 20.529	-0.721	1.00	88.70
	1485	O6	NAG	166B	9.186	20.52 5 22.047	-4.475	1.00	140.23
20	1486	C1	MAN	166C	7.210	23.248	-3.529	1.00	140.23
20	1487	C2	MAN	166C	6.971	23.629	-2.897	1.00	140.23
	1488	02	MAN	166C	8.186	24.444	-4.292	1.00	140.23
	1489	СЗ	MAN	166C	6.384 7.294	24.880	-5.294	1.00	140.23
	1490	O 3	MAN	166C	7.294 5.054	24.047	-4.942	1.00	140.23
25	1491	C4	MAN	166C 166C	4.019	24.073	-3.966	1.00	140.23
	1492	O4	MAN			22.640	-5.572	1.00	140.23
	1493	C5	MAN	166C 166C		22.236	-5.734	1.00	140.23
	1494	O 5	MAN	166C		22.590	`-6. 94 6	1.00	140.23
	1495	C6	MAN	166C		21.313	-7.207	1.00	140.23
30	1496	06	MAN WAT	1000		20.612	-1.007	1.00	68.91 68.91
	1497	OH2	WAT	1001		15.888	-2.154	1.00	68.91
	1498	OH2	WAT	1002		8.073	7.063	1.00	68.91
	1499	OH2	WAT	1003		3.262	-1.304	1.00 1.00	68.91
0.5	1500	OH2 OH2	WAT	1004		-6.784	-6.997	1.00	68.91
35	1501	OH2	WAT	1005		-7.978	-9.801	1.00	68.91
	1502	OH2	WAT	1006		-8.042	14.310 -0.296	1.00	68.91
	1503	OH2	WAT	1007		5.554	12.004	1.00	68.91
	1504 1505	OH2	WAT	100		2.758	2.679	1.00	68.91
40		OH2	WAT	100		17.603	-7.289		68.91
	1507	OH2	WAT	101		14.371 -2.803	0.523		68.91
\	1508	OH2	TAW	101	1 29.583	-6.190	4.824		68.91
	1509	OH2	WAT	101		4.228	29.002		68.91
	1510	OH2	WAT	101		19.173	25.674		68.91
45	1511	OH2	WAT	101		-12.922	-8.874		68.91
	1512	OH2	WAT	101		0.066	-4.940	1.00	68.91
	1513	OH2	WAT	101		10.290	21.60	5 1.00	68.91
	1514	OH2	WAT	101 101		12.690	26.479	9 1.00	68.91
	1515	OH2	TAW	10		28.860	10.13		68.91
50		OH2	WAT	10	• • • • • • • • • • • • • • • • • • • •		3.31		68.91 68.91
	1517	OH2	TAW TAW	10			-2.75		68.91
	1518	OH2	WAT	10			-10.50		68.91
	1519	OH2	WAT		23 26.056	0.085	8.31		68.91
-	1520	OH2 OH2			24 29.558	14.948	9.23		68.91
2	5 1521	OH2			25 28.174		-11.72		68.91
	1522	OH2			26 9.612	1.088	0.70		68.91
	1523	OH2			27 28.026	4.309	20.41		68.91
	1524 1525	OH2			28 25.503	9.375	10.44 -7.39		68.91
	50 1526	OH2	·	10	29 16.927		-7.33 32.04		68.91
,	1527	OH2			32.00		21.2		68.91
	1528		WAT		031 12.4		19.1		68.91
	1529		WAT		032 15.32		33.9		
	1530			1	033 11.53	0.204	55.5		

	4504	OH2	WAT	1034 - 18.003	7.978	-6.726	1.00	68.91
	1531		WAT	1035 34.477	2.731	-7.719	1.00	68.91
	1532	OH2	WAT	1036 25.373	34.820	8.269	1.00	68.91
	1533	OH2 OH2	WAT	1037 14.026	16.389	25.301	1.00	68.91
5	1534	OH2	WAT	1038 30.733	30.153	16.022	1.00	68.91
2	1535		WAT	1039 25.276	21.121	-10.191	1.00	68.91
	1536	OH2	WAT	1040 16.971	8.768	-11.221	1.00	68.91
	1537	OH2	WAT	1040 10.571	12.580	36.282	1.00	68.91
	1538	OH2		1041 20.557	6.575	17.557	1.00	68.91
••	1539	OH2	WAT WAT	1042 5.334	-14.196	14.154	1.00	68.91
10	1540	OH2		1043 20.423	6.111	-5.021	1.00	68.91
	1541	OH2	WAT	1045 16.712	8.152	1.031	1.00	68.91
	1542	OH2	WAT	1045 10.712	17.172	0.994	1.00	68.91
	1543	OH2	WAT	1046 10.222	8.260	28.436	1.00	68.91
	1544	OH2	WAT		12.929	2.834	1.00	68.91
15	1545	OH2	WAT	1048 17.529 1049 31.571	12.227	-10.072	1.00	68.91
	1546	OH2	WAT		1.995	35.016	1.00	68.91
	1547	OH2	WAT	1050 22.536	6.724	-12.642	1.00	68.91
	1548	OH2	WAT	1051 26.121	0.724	2.327	1.00	68.91
	1549	OH2	WAT	1052 14.788	12.151	-8.959	1.00	68.91
20	1550	OH2	WAT	1053 36.387	-9.146	-4.152	1.00	68.91
	1551	OH2	WAT	1054 30.213	21.863	-0.263	1.00	68.91
	1552	OH2	WAT	1055 33.615	-4.295	32.761	1.00	68.91
	1553	OH2	WAT	1056 10.283	-4.295 0.501	-14.456	1.00	68.91
	1554	OH2	WAT	1057 28.514		16.354	1.00	68.91
25	1555	OH2	WAT	1058 16.608	-5.089 0.749	2,548	1.00	68.91
	1556	OH2	WAT	1059 32.212	-2.748	-6.1 93	1.00	68.91
	1557	OH2	WAT	1060 28.253	-14.928	20.937	1.00	68.91
	1558	OH2	WAT	1061 22.375	14.011	18.605	1.00	68.91
	1559	OH2	WAT	1062 17.962	-4.643 17.614	12.726	1.00	68.91
30	1560	OH2	WAT	1063 33.412	17.614	5.224	1.00	68.91
	1561	OH2	WAT	1064 14.403	13.829	22.648	1.00	68.91
	1562	OH2	WAT	1065 22.334	16.845 -0.489	7.854	1.00	68.91
	1563	OH2	WAT	1066 3.946		5.1 89	1.00	68.91
	1564	OH2	WAT	1067 19.383	17.873	23.054	1.00	68.91
35	1565	OH2	WAT	1068 15.472	16.647	2.954	1.00	68.91
	1566	OH2	WAT	1069 29.541	28.573	32.823	1.00	68.91
	1567	OH2	WAT	1070 22.439	9.086	4.613	1.00	68.91
	1568	OH2	WAT	1071 12.994	2.582	4.759	1.00	68.91
	1569	OH2	WAT	1072 8.173	-4.098	-8.5 63	1.00	68.91
40	1570	OH2	WAT	1073 6.843	21.529 8.743	13.308	1.00	68.91
	1571	OH2	WAT	1074 6.493		-0.320	1.00	68.91
	1572	OH2	WAT	1075 38.018	4.521	18.115	1.00	68.91
	1573	OH2	WAT	1076 24.471	-3.010	10.596	1.00	68.91
	1574	OH2	WAT	1077 25.888	-4.454 7.299	-5.712	1.00	68.91
45	1575	OH2	WAT	1078 14.459		11,601	1.00	68.91
	1576	OH2	WAT	1079 29.390	19.413	28.950	1.00	68.91
	1577	OH2	WAT	1080 20.808	23.774			68.91
	1578	OH2	WAT	1081 30.321	32.666	4.517 5.513	1.00 1.00	68.91
	1579	OH2	WAT	1082 18.638	14.702	24.212	1.00	68.91
50	1580	OH2	WAT	1083 10.393	2.751		1.00	68.91
	1581	OH2	TAW	1084 34.357	8.750	4.350	1.00	აგ.91
	1582	OH2	TAW	1083 38.981	27.376	6.226	1.00	68.91
	1583	OH2	WAT	1086 13.633	-5.771	10.421	1.00	68.91
	1584	OH2	WAT	1087 30.187	-0.118	1.986		68.91
55	1585	OH2	WAT	1088 19.984	12.423	13.551 3.694	1.00 1.00	68.91
	1586	OH2	WAT	1089 33.138	0.672			68.91
	1587	OH2	WAT	1090 22.605	13.264	0.581 9.575	1.00	68.91
	1588	OH2	WAT	1091 14.668	10.306	8.575	1.00	68.91
	1589	OH2	WAT	1092 21.896	16.105	11.480	1.00	68.91
60	1590	OH2	TAW	1093 26.996	0.604	11.132	1.00	
	1591	OH2	WAT	1094 31.571	7.546	16.430	1.00	68.91
	1592	OH2	WAT	1095 30.193	3.267	-18.033	1.00	68.91 68.91
	1593	OH2	TAW	1096 30.112	6.862	20.521	1.00	68.91
	1594	OH2	WAT	1097 25.159	32.416	11.157	1.00	00.31

1595 1596 1597 1598 5 1599 1600 1601 1602 1803 10 1604 1605 1606	OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2 OH2	WAT	1098 - 25.354 1099 20.969 1100 32.515 1101 30.357 1102 30.517 1103 13.656 1104 15.222 1105 34.184 1106 27.056 1107 33.492 1108 12.951 1109 23.498	-13.410 -1.882 -1.311 10.302 8.184 -2.654 19.539 25.830 25.512 6.985 8.497 11.331	18.368 24.389 -2.770 -14.689 27.857 31.941 18.640 5.139 13.333 -2.929 11.009 13.153 18.238	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91
1607 1608 15 1609 1610 1611 1612 1613 20 1614 1615 1616 1617 1618 25 1619 1620	OH2	WAT	1110 29.557 1111 29.239 1112 20.316 1113 27.872 1114 21.439 1115 34.052 1116 11.123 1117 10.985 1118 33.767 1119 23.247 1119 31.382 1120 31.382 1121 12.025 1122 9.969 1123 20.360	-10.045 18.077 12.553 2.853 20.739 2.985 -3.141 13.263 28.659 24.523 23.627 -1.649 2.385 -3.059	-10.203 -11.333 -33.575 -11.349 -36.842 -18.133 -12.061 -2.115 -18.586 -14.310 -0.565 -20.835 -13.904	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91 68.91

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As used herein, an atomic coordinate, also referred to herein as a structure coordinate or coordinate, is a mathematical coordinate derived from mathematical equations related to the patterns obtained on diffraction of X-rays by the atoms of a protein crystal. The diffraction data are typically used to calculate an electron density map, such as that shown in Fig. 1, which is used to establish the positions of the individual atoms within the unit cell of the crystal. A model that substantially represents the atomic coordinates specified in Table 1 includes not only models that literally represent the coordinates but also models representing a coordinate transformation of such atomic coordinates, for example, by changing the spatial orientation of the coordinates.

- 1₄ (1, 3)

Additional embodiments of the present invention include 3-D models of extracellular domains of FceRI\alpha proteins that substantially represent the atomic coordinates specified in Table 5, Table 6, Table 7 or Table 8, each of which is at the end of the Examples section. Similarly, a model that substantially represents the atomic coordinates specified in Table 5, Table 6, Table 7 or Table 8 includes not only models that literally represent the coordinates but also models representing a coordinate transformation of such atomic coordinates.

The present invention also includes a 3-D model that is a modification of a 3-D model that substantially represents the atomic coordinates specified in Table 5, Table 6, Table 7 or Table 8. As used herein, a modification, also referred to herein as a model modification, is a model that represents a protein that binds to a Fc domain of an antibody. A model modification includes, but is not limited to: a refinement of the model that substantially represents the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8; a model representing any fragment of a protein having the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8 that binds to a Fc domain of an antibody; a model based on other FceRIa protein crystals, such as a model based on one or more of the crystals disclosed in the Examples; a model produced using homology modeling techniques to, for example, incorporate all or any part of the amino acid sequence of another FcR into a 3-D model of the extracellular domain of the model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8 or incorporate all or any part of the amino acid sequence of a FceRIa protein into a 3-D model of another FcR; and a modification representing a FcR 30

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with an altered function, which preferably can be used to design a mutein with an improved function compared to an unmodified protein. As used herein, the term unmodified protein refers to a protein that has not been intentionally subjected to either random or site-directed (i.e., targeted) mutagenesis.

A model of the present invention can be represented in a variety of forms including, but not limited to, listing the coordinates of all atoms comprising the model, providing a physical 3-D model, imaging the model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of the model, for example by extracting coordinates from a picture or placing a similar immunoglobulin domain into the 3-D model of human $FeeRIa_{1-176}$ protein form M1, FceRI α_{1-176} protein form M2, FceRI α_{1-172} protein form T1, FceRI α_{1-172} protein form T2, or $FceRI\alpha_{1-172}$ protein form H1 and deriving a model of the similar domain. Physical 3-D models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, Biosym Technologies, San Diego, CA, Tripos, Inc., and Molecular Simulations Inc. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Hard copies include both motion and 20 still pictures. Computer screen images and pictures of the model can be visualized in a number of formats including, but not limited to, electron density maps, ribbon diagrams, space-filling representations, α carbon traces, topology diagrams, lists of interatomic vectors, phi/psi/chi angle representations of the coordinates, and contact maps, examples of some of which are in the Figs. Representations of the model can include the entire model or portions thereof.

In one embodiment, a model of the present invention identifies the solvent accessibility of amino acid residues of the corresponding protein. The solvent accessibilities of the amino acids in human FceRI α_{1-176} protein (form M1) are indicated in Table 2.

Table 2. PhFceRIa₁₋₁₇₆, Form M1, residue exposure

>>>> Surface plot for:
>>>> structure file= fcr10_gen.mtf
>>>> coordinate set= fcr10b.pdb

	>>>>			access-main	access-side
5	resid	resname	access	access-main	
•			40.7500	5.5920	29.2803
	4	LYS	18.7522	0.7105	0.2895
	5	PRO	0.5301	0.5227	25.5856
	6	LYS	14.4465	2.9151	0.0000
	7	VAL	1.6658	1.6199	28.7895
10	8	SER	10.6765	4.3765	2.4038
	9	LEU	3.3901	0.9379	24.0120
	10	ASN	12.4750	0.1890	21.0688
	11	PRO	9.1378	2.5914	21.7181
	12	PRO	10.7886	0.1461	3.8672
15	13	TRP	2.8040	0.0019	5.6746
	14	ASN	2.8382	0.0047	1.3672
	15	ARG	0.8717	0.0000	1.6524
	16	ILE	0.8262	0.0002	0.3536
	17	PHE	0.2251	2.1781	16.8470
20	18	LYS	10.3275	5.9941	0.0000
	19	GLY	5.9941	0.0003	6.2230
	20	GLU	3.4574	3.1911	7.8142
	21	ASN	5.5027	0.5396	0.2464
	22	VAL	0.4139	0.0611	12.3812
25		THR	5.3412	0.0000	0.2767
	24	LEU	0.1383	0.0105	16.1931
	25	THR	6.9459	0.2962	0.0913
	26	CYS	0.2279	2.3608	10.3594
	27	ASN	6.3601	15.2937	0.0000
30	0 28	GLY	15.2937	3.3134	21.8538
_	29	ASN.	12.5836	4.7397	1.1246
	30	ASN	2.9321	0.4808	16.9384
	31	PHE	10.9538	5.7840	23.2409
	32	PHE	16.8929	11.1422	26.0256
3	5 33	GLU	19.4108	4.6702	18.8072
	34	VAL	10.7289	2,0900	3.0905
	35	SER	2.4235	6.2435	28.9679
	36	SER	13.8183	0.0825	0.3679
	37	THR	0.2048	0.0996	19.7850
	40 38	LYS	11.0359	0.0000	0.0311
	39	TRP	0.0222	0.0194	4.9894
	40	PHE	3.1821	0.3964	5.3667
	41		3.3786 6.4876	7.0690	5.9062
	42	ASN	0.4070	10.7019	0.0000
	45 43	GLY	10.7019	1.4355	32.3926
	44	SER	11.7545	7,2235	18.3003
	45	5 LEU	12.7619	3.6359	8.2137
	40		5.1618	6.7955	28.6039
	4		18.9113	1.8435	7.8693
	50 4	B GLU	5.1912	0.7172	23.5005
	4		10.4814	1.2937	
	5	0 ASN	12.2883	,.200.	

			7.5408	0.9771	20.6683
5		SER	5.9824	1.1729	15.6016
5		SER	2.7948	0.0000	5.5895
	3	LEU	11.0365	4.8824	17.1907
	i4	ASN	1.4787	1,1377	1.8197
	55	ILE	10.1929	3.7822	18.7406
	56	VAL	10.1929	0.9161	19.1928
	57	ASN	0.4355	0.5444	0.0000
	58	ALA	12.3709	0.0000	22.2676
	59	LYS	3.8585	0.0995	6.0065
	60	PHE	8.4358	0.0765	15.1232
	61	GLU	3.5771	0.0000	7.1543
	62	ASP	0.1109	0.0000	0.3328
	63	SER	1.4454	1.4454	0.0000
	64	GLY	3.8623	0.1172	6.8583
15	65	GLU TYR	0.6305	0.0000	0.9458
	66		5.0231	0.0000	9.0416
	67	LYS CYS	0.0000	0.0000	0.0000
	68	GLN	4.0004	0.1217	7.1034
	69	HIS	1.6360	1.2124	1.9183
20	70	GLN	12.0520	6.5738	16.4346
	71	GLN	6.9718	4.8885	8.6385
	72	VAL	18.2550	4.0583	37.1841
	73	ASN	11.7258	0.8064	22.6451
25	74 75	GLU	8.0572	4.5805	10.8386
25	75 76	SER	1.1935	1.7903	0.0000
	76 77	GLU	11.7837	0.3001	20.9705
	77 78	PRO	6.8729	3.9043	10.8310
	78 79	VAL	4.7487	0.8978	9.8832
30	80	TYR	10.6722	1.0753	15.4707 0.3678
30	81	LEU	0.6889	1.0101	10.8066
	82	GLU	6.0039	0.0005	0.0000
	83	VAL	1.1805	2.0660	4.5925
	84	PHE	3.1391	0.5957	19.7676
35	85	SER	11.3103	7.0817	8.2880
33	86	ASP	5.0469	1.8059	12.3027
	87	TRP	8.7876	0.0000	0.0000
	88	LEU	0.2129	0.4258	0.9408
	89	LEU	0.4967	0.0525 0.0599	0.0000
40	90	LEU	0.0300	0.0000	0.3323
	91	GLN	0.1846	0.0000	0.0495
	92	ALA	0.1116	5.5213	8.8700
	93	SER	6.6376	1.3918	28.7952
	94	ALA	6.8725	1.6594	11.9535
45	95	GLU	7.3784	3.7388	22.0772
	96	VAL	11.5981	0.7102	0.9951
	97	VAL	0.8323	0.4727	22.0682
	98	MET	11.2704	2.3489	14.3246
	99	GLU	9.0020	8.7203	0.0000
50		GLY	8.7203	0.0000	19.0137
	101	GLN	10.5632 7.5364	2.1046	14.7788
	102		7.53 04 0.0101	0.0065	0.0136
	103		7.5886	0.0000	11.9250
_	104		0.0013	0.0000	0.0026
5	5 105		5.0182	0.0005	7.8855
	106	ARG	3,0,02		

			0.4060	0.1901	0.0004
	107	CYS	0.1269 0.9132	0.3845	1.2657
	108	HIS	0.5179	0.5179	0.0000
	109	GLY	4.56 9 0	0.0000	6.3966
	110	TRP	16.0050	8,4847	20.3023
5	111	ARG	12.3469	5.3472	19.3466
	112	ASN	5.4418	2.5536	6.5971
	113	TRP		2.6722	21.8150
	114	ASP	12.2436	1.1789	0.9745
	115	VAL	1.0913	0.0536	14.9114
10	116	TYR	9.9588	6.4497	23.3321
• •	117	LYS	15.8288	3.9634	0.3269
	118	VAL	2.4049	0.0000	14.9016
	119	ILE	7.4508	0.0000	0.0000
	120	TYR	0.0000	0.0193	5.2936
15	121	TYR	3.5355	0.3398	8.1440
	122	LYS	4.6755	6.7061	13.6465
	123	ASP	10.1763	13.3789	0.0000
	124	GLY	13.3789	0.9044	23.0796
	125	GLU	13.2240	3.5091	35.0725
20	126	ALA	9.8218	3.0445	2.6843
20	127	LEU	2.8644	8.2304	29,4606
	128	LYS	20.0249	2.8367	12.5774
	129	TYR	9.3305	6.2307	20.5908
	130	TRP	16.4879	3,5735	3.3740
25	131	TYR	3.4405	2.0563	19.7905
ديد	132	GLU	11.9086	4,2727	14.2802
	133	ASN	9.2765	0.0000	12.7321
	134	HIS	7.6393	0.1229	15.8860
	135	ASN	8.0044	0.1229	0.4205
30		ILE	0.3804	6.1883	17.4541
50	137	SER	9.9436	0.9189	1.0252
	138	ILE	0.9720	2.3046	30.6869
	139	THR	14.4684	3,2729	22.0554
	140	ASN	12.6642	0.2930	0.0431
3.		ALA	0.2430	0.0000	15.8087
٠.	142	THR	6.7751	1.2997	31.8640
	143	VAL	14.3987	2.9912	23.5929
	144	GLU	14.4366	0.0018	1.2841
	145	ASP	0.6429	1.9108	12.8352
Δ	0 146	SER	5.5523	4.1321	0.0000
_	147	GLY	4.1321		9.5879
	148	THR	4.1370	0.0488 0.0000	0.0398
	149		0.0265	0.0000	5.7220
	150		3.8147	0.0000	0.0000
	45 151		0.0000	0.0000	8.6747
	152		3.7177	0.4224	0.0000
	153		0.4224	-	11.3765
	154		6.3203	0.0000 0.0267	0.0620
	15		0.0418		15.2367
	50 15		11.9658	3.7888	24.2849
	15		15.4277	4.3561	27.8104
	15		14.1140	0.4176	19.8215
	15		13.2798	6.7381	5.2517
	16	~	4.2173	2.1486	17.4267
	55 16		11.5466	4.1966	0.0000
	16		0.5960	0.8940	0,0000
	10				

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		0111	10.5746	0.2964	18.7972
	163	GLU	11.0115	3.8863	20.5117
	164	PRO	1.6740	0.6758	2.6721
	165 .	LEU	5,2259	2.2692	8.1825
	166	ASN		0.5937	0.0000
5	167	ILE	0.2968	0.0262	22.8875
	168	THR	9.8239	2.6882	0.3236
	169	VAL	1.6748	1.8982	18.8869
	170	ILE	10.3926		25.3128
	171	LYS	15.1729	2.4981	43.7220
10	172	ALA	11.6822	3.6722	24.1346
	173	PRO	13.4157	5.3766	28.6460
	174	ARG	25.5533	20.1410	17.8283
	21A	NAG	17.8283	0.0000	
	42A	NAG	10.6799	0.0000	10.6799
15	42B	NAG	8.9040	0.0000	8.9040
15	42C	MAN	17.4386	0.0000	17.4386
	166A	NAG	16.8280	0.0000	16.8280
		NAG	16.9174	0.0000	16.9174
	166B	MAN	21.1827	0.0000	21.1827
	166C	IAIVIA			

The solvent accessibilities of the amino acids in human FceRIα protein forms T1, T2, M2 and M1 are indicated in Tables 9, 10, 11, and 12 respectively, each of which is at the end of the Examples section.

Residues that are solvent accessible are important as they represent amino acids that are on the external surface of the protein and, as such, may be involved in binding of a FcR to an antibody and as such be useful in designing proteins with an enhanced binding activity or in identifying compounds that inhibit such binding. In addition, solvent accessible residues can represent targets for modification to produce a FcR with improved function. Such analysis also identifies residues in the interior, or core, of the protein. Such residues can also be targeted to produce proteins with improved functions, such as enhanced stability. A model of the present invention also provides additional information that is not available from other sources. For example, a model can identify the crystal contacts between crystals and predict the location of the IgE binding domain, including those amino acids that actually form contacts with a Fc domain of an IgE antibody, such as those in the binding face of the FceRla protein. A model can also identify the amino acids in the interface between domain 1 and domain 2 (i.e., the D1D2 interface), as well as those in the cleft formed between the two domains.

One embodiment of the present invention is a model that represents a protein that binds to a Fc domain of an IgE antibody with an affinity that is at least equivalent to the affinity of the extracellular domain of human FcεRlα for any one of the following IgE antibodies: a human IgE antibody, a canine IgE antibody, a feline IgE antibody, an equine IgE antibody, a rat IgE antibody, and a murine IgE antibody. Such a model can represent an extracellular domain of a human FcεRlα protein, a canine FcεRlα protein, a feline FcεRlα protein, an equine FcεRlα protein, a murine FcεRlα protein, and a rat FcεRlα protein. Such a model can also represent a protein with altered substrate specificity, preferably designed based on a model of the present invention. WO 98/23964, *ibid.*, reports the ability of an isolated human FceRlα protein to bind to canine, feline and equine IgE antibodies. Models of the present invention can be used to design a FcR with increased affinity for an antibody of a species other than self, such as, but not limited to, a human FceRlα with increased affinity for a canine, feline or equine IgE antibody.

The present invention includes a model that represents a FcR that binds to an antibody of its respective class (i.e., IgE, IgG, IgM, IgA or IgD antibody class). Also included is a model that represents a FcR designed to bind to an antibody of a class other than the class to which the protein naturally binds. Such a model of the present invention can be produced, for example, by incorporating all or any part of the amino acid sequence of the other FcR into a 3-D model of the extracellular domain of a human FceRIa protein. Such an embodiment includes any model that specifically incorporates any Ig domains that are placed in an orientation (packing interfaces and bend angles) that is based on the structure of the FceRIa. A preferred model of the present invention represents a FcR that binds to an IgE antibody or to an IgG antibody. In one embodiment, a model of the present invention is a 3-D model of an extracellular antibody binding domain of a FcR other than human FceRIa, such as of a FcR that binds to an IgG antibody. Such proteins and models thereof can be designed by homology modeling by, for example, altering the substrate specificity of a FceRIa protein such that the altered protein binds an IgG antibody.

A preferred modified model of the present invention is a model that has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstrom when superimposed, using backbone atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7 or Table 8, and more particularly atomic coordinates specified in Table 1. Preferably such a model has a 3-D structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 8 angstroms, preferably less than 7 angstroms, preferably less than 6 angstroms, preferably less than 5 angstroms, preferably less than 4 angstroms, preferably less than 3 angstroms, preferally less than 2 angstroms, and preferably less than 1 angstroms, when superimposed, using backbon3 atoms, on the 3-D model substantially represented by the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8, and more particularly atomic coordinates specified in Table 1. In this embodiment, such a model represents a FcR that binds to an antibody. The backbone atoms are those atoms that form the backbone, or 3-D folding pattern, of the model. As such, backbone atoms are the base residues of amino acids, i.e., nitrogen, carbon, the alpha carbon and oxygen.

Also preferred is a model modification having an amino acid sequence that shares at least about 30%, preferably at least about 40%, more preferably at least about 45%, more preferably at least about 50%, more preferably at least about 60% and even more preferably at least about 80% amino acid sequence homology, with a human FcεRIα protein, as determined using the program ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts. It is to be noted that, using the same program and parameters, the extracellular domain of a human FcεRIα protein (i.e., soluble human FcεRIα protein) shares about 48% identity with feline and rat soluble FcεRIα proteins, about 49% with a murine soluble FcεRIα protein, about 50% identity with a canine soluble FcεRIα protein, and about 60% identity with an equine soluble FcεRIα protein. A preferred model of the present invention represents an IgE binding domain, i.e., a region that binds to an IgE antibody.

One embodiment of the present invention is a 3-D model of a human FceRIa protein produced by a method that includes the steps of: (a) crystallizing an extracellular domain of a human FceRIa protein, such as, but not limited to a protein having amino acid sequence SEQ ID NO:2 or SEQ ID NO:4; (b) collecting X-ray diffraction data from the crystallized protein; and (c) determining the model from the X-ray diffraction data, preferably in combination with an amino acid sequence of the protein. A protein for crystal formation can be produced using a variety of techniques well known to those skilled in the art. As disclosed herein, a human FceRIa protein to be crystallized is preferably produced in recombinant insect cells transformed with a gene encoding an extracellular domain of a human FceRIa protein, such as a baculovirus genetically engineered to produce the protein. The purity of the FceRIa protein must be sufficient to permit the production of crystals that can be analyzed by X-ray crystallography to a resolution that permits determination of a 3-D model of the protein. Preferably the resolution is at least about 4 angstroms (i.e., 4 angstroms or better), more preferably at least about 3.5 angstroms, more preferably at least about 3 angstroms, more preferably at least about 2.5 angstroms, more preferably at least about 2 angstroms and even more preferably at least about 1.5 angstroms. Methods to obtain such purity levels are well known to those skilled in the art.

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As disclosed herein, a preferred method to crystallize a FceRIa protein is by vapor distillation. Particularly preferred methods are disclosed in the Examples. It should be appreciated that the present invention also includes other methods known to those skilled in the art by which the protein can be crystallized.

3-D models of some proteins have been determined; see, for example, Blundell et al., *Protein Crystallography*, Academic Press, London, 1976. However, as discussed herein, elucidation of the crystal structure of the extracellular domain of the human FceRIa was difficult. In one embodiment, crystal structure determination includes obtaining high-resolution data using synchrotron radiation. Such data can be collected, for example, at the Stanford Synchrotron Source Laboratory, Palo Alto, CA, or the Advanced Photon Source at Argonne National Laboratories, Argonne, IL. Additional locations to collect such data include, but are not limited to, Brookhaven, NY, and Japan. In one embodiment, diffraction data from native and heavy-atom treated crystals provide an initial image of the protein structure which is refined into an electron density map. Details regarding data collection and interpretation are provided in the Examples section.

One embodiment of the present invention is a method to produce a 3-D model of a FceRI\(\alpha\) protein that includes positioning amino acid representations (i.e., representing amino acids) of the protein at substantially the coordinates listed in Table 1, Table 5, Table 6, Table 7, or Table 8. That is, knowledge of the coordinates of the protein permits one skilled in the art to produce a model of the protein using those coordinates. Such a model, or any model which is essentially represented by a simple coordinate transformation of the coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8, can be represented in a variety of methods as heretofore disclosed and is included in the present invention.

In another embodiment, a model of the present invention can be refined to obtain an improved model, which is an example of a model modification, also referred to as a modified model. Refining methods can include, but are not limited to, further data collection and analysis; data collection from frozen crystals; introduction of solvent molecules to the structure; clarification of secondary structure; and analyses of crystallized complexes between a FcR and an antibody or inhibitory compound. An

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additional model refinement method includes analyzing a 3-D model to predict amino acid residues that if replaced are likely to yield proteins with at least one improved function, effecting at least one such replacement, determining whether the activity of the modified protein agrees with the prediction, and refining the model as necessary.

Methods to determine whether the modification agrees with prediction include producing the modified protein and performing assays with that modified protein to determine if the protein does indeed exhibit the improved function(s), such as desired activity, stability and solubility properties. Assays to measure such functions are well known in the art; examples of several such assays are disclosed herein.

Another embodiment of the present invention is a modified 3-D model that represents a FcR other than a human FceRIa protein represented by the 3-D model the coordinates of which are listed in Table 1, Table 5, Table 6, Table 7, or Table 8. Preferably the amino acid sequence of the protein to be modeled is known. In such a case, the modified model can be produced using the technique of homology modeling, preferably by incorporating (e.g., grafting, overlaying or replacing) all or any portion of the amino acid sequence of the other FcR into the 3-D model of the human FceRIa protein to produce the modified model which comprises the other FcR. General techniques for homology modeling, also referred to as molecular replacement, have been disclosed in, for example, Greer, 1990, Proteins: Structure, Function, and Genetics 7, 317-334; Havel et al., 1991, J. Mol. Biol. 217, 1-7; Schiffer et al., 1990, Proteins: Structure, Function, and Genetics 8, 30-43; and Lattman, 1985, Methods Enzymol 115, 55-77. However, such technology has not been applied to FcRs since, until the present invention, no 3-D model of any FcR was available. Thus, the present invention now allows the solving of the structures of a number of other natural and mutated forms of FcRs or any other protein with significant amino acid homology, especially to the 25 functional Ig domains of the human FceRIa protein.

In one embodiment, a model of a FcR, such as, but not limited to a FceRI α protein, is produced by extracting the 3-D coordinates from a published figure or building a 3-D model with atoms from other Ig domains wherein the Ig domains are oriented as predicted for a human FceRI α_{1-176} protein or a FceRI α_{1-172} protein. For example, a model of the present invention can be produced by orienting two known Ig

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domains into a bent confirmation similar to that of the two domains of the human FceRIa protein. Such a model is referred to as a model in which domain 1 and domain 2 are oriented in a manner as specified by the structural coordinates listed in Table 1, Table 5, Table 6, Table 7, or Table 8. This model can then be used in further molecular replacement methods. Such methods can include the steps of (a) orienting the model by three rotations; and (b) translating the model in one to three directions to produce additional model modifications.

Suitable FcRs for which a 3-D model can be determined using homology modeling include any mammalian FcR, such as a protein that binds to IgE, IgG, IgM, 10 IgA or IgD antibodies. Preferred is a protein that binds to an IgE antibody or an IgG antibody. Preferred FcRs that bind to IgE include human, canine, feline, equine, murine and rat FceRIa proteins. The present invention also includes the use of other Ig domains to produce models of the present invention.

One embodiment of the present invention is a 3-D model of a FcR having an improved function compared to an unmodified protein as well as a method to produce such a modified model. Such an improved function includes, but is not limited to, enhanced activity, enhanced stability and enhanced solubility. Such a modified model can be produced by replacing at least one amino acid based on information derived from analyzing the 3-D model of a FceRI α protein, such as the model of a human FceRI α_{1-176} protein or a $FceRI\alpha_{1-172}$ protein, such that the replacement leads to a protein with an improved function. As used herein, a replacement refers to an (i.e., one or more) amino acid substitution, insertion, deletion, inversion and/or derivatization (e.g., acetylation, glycosylation, phosphorylation, PEG modification, biotinylation, and covalent attachment of other ligands or other compounds to the protein. In one embodiment, synthetic chemical methods are used to produce either a fragment or the entire protein to, 25 for example, introduce non-natural amino acids or other chemical compounds into the structure of a FcR. For example, based on a structure of the present invention, one can design synthetic peptides or larger proteins that could be linked to produce an intact protein with IgE binding activity, the structure allowing one to design the start and stop points for these peptides, e.g., at surface accessible loops. In accordance with the present invention, an amino acid that is substituted or inserted can be a natural amino

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acid or an unnatural amino acid, including a derivitized amino acid. Methods to identify regions in the protein that, if changed, yield a protein with an improved function are disclosed below.

The present invention includes use of a 3-D model of the present invention to identify a compound that inhibits binding between a box and an antibody. The advantages of using a 3-D model to identify inhibitory compounds are multi-fold in that the model depicts the site at which a Fc domain of an antibody binds to its FcR, i.e., the antibody-binding domain, also referred to as the antibody binding site. As such, a large number of potential inhibitory compounds can be initially analyzed without having to perform in vitro or in vivo laboratory studies. As used herein, methods to identify inhibitory compounds include, but are not limited to, designing inhibitory compounds 10 based on the 3-D model of a FcR, probing such a 3-D model with compounds that are potential inhibitors in order to identify those compounds that are actually inhibitory of the binding of an antibody to its FcR, screening a compound data base using such a 3-D model to identify compounds that inhibit such binding, and combinations thereof. Methods to use 3-D models to design, probe for, or screen for suitable inhibitory 15 compounds are known to those skilled in the art. In particular, there are a number of computer programs that enable such methods. See, for example, PCT Publication No. WO 95/35367, by Wilson et al., published December 28, 1995.

An inhibitory compound can be any natural or synthetic compound that inhibits the binding of an antibody to a FcR. Examples include, but are not limited to, inorganic compounds, oligonucleotides, proteins, peptides, antibodies, antibody fragments, mimetics of peptides or antibodies (such as, mimetics of antibody or receptor binding sites), and other organic compounds. Compounds can inhibit binding in either a competitive or non-competitive manner and can either interact at the binding site or allosterically. An inhibitory compound should be capable of physically and structurally associating with a FcR and/or an antibody such that the compound can inhibit binding between the two entitites. As such, an inhibitory compound is preferably small and is of a structure that effectively prevents or disrupts binding. Inhibitory compounds can be identified in one or multiple steps. For example, a compound initially identified that inhibits binding between an antibody and FcR to some extent can be used as a lead to

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design, probe or screen for a compound with improved characteristics, such as greater efficacy, safety, solubility, etc. A preferred inhibitory compound is a compound that is efficacious when administered to an animal in an amount that results in a serum concentration of from about 1 nanomolar (nM) to 100 micromolar (µM), with a concentration of from about 10 nM to 10 μ M being more preferred.

One embodiment of the present invention is a method to identify a compound that inhibits the binding between an IgE antibody and a FceRIa protein. Such a method includes the step of using a 3-D model substantially representing the atomic coordinates specified in T_{ϵ} le 1, Table 5, Table 6, Table 7, or Table 8 to identify such a compound. Included in the present invention are inhibitory compounds that interact directly with the IgE binding domain or the receptor binding domain of the IgE antibody as well as compounds that interact indirectly with an FceRIa protein, such as compounds that interact with the D1D2 interface, with the cleft between D1 and D2, with a region not consisting of a N-linked glycosylation site, with a region suggested by a combination of 3-D model and mutagenesis analysis to indirectly affect antibody binding, a region suggested by homology with other FceRIa proteins of other species, a region suggested 15 by homology with other FcRs. In a preferred embodiment, an inhibitory compound interacts with at least one of the following regions of a model representing a FceRIa protein: a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, a C'E loop of D2, a F strand of domain D2, a FG loop of D2, and a tryptophan-containing hydrophobic ridge. It is to be noted that the A'B and EF loops of 20 D1 are immediately adjacent to the IgE binding domain in D2 and as such are predicted, for the first time, by the model to be good targets for inhibitory compounds. In a preferred embodiment, an inhibitory compound of the present invention interacts with at least one amino acid that is a crystal contact as predicted by the atomic coordinates listed in Table 1, Table 5, Table 6, Table 7 or Table 8. Inhibitory compounds of the present 25 invention preferably interact with at least one of the following amino acid residues: amino acid 87, 110, 113, 115, 117, 118, 120, 121, 122, 123, 128, 129, 131, 149, 153, 154, 155, 156, 157, 158, and 159 of SEQ ID NO:2 or SEQ ID NO:4, as well as any surface residue within about 10 angstroms of any of the listed amino acids. More 30

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preferred is an inhibitory compound that interacts with at least one amino acid that is a crystal contact predicted to also be part of the IgE binding domain. Particularly preferred are amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4. In one embodiment, an inhibitory compound of the present invention is a peptide corresponding to at least a portion of any of the identified regions or a derivative thereof, such as a peptide mimetic or other compound that mimics that peptide. Preferred is a peptide corresponding to at least a portion of the FG loop of D2, or a derivative thereof, such as a peptide mimetic or other compound that mimics that peptide. 10

One embodiment of a method to identify a compound that inhibits the binding between an IgE antibody and a FceRIa protein includes the steps of: (a) generating a model substantially representing the atomic coordinates listed in Table 1, Table 5, Table 6, Table 7, or Table 8, or a model of an IgE binding domain thereof, on a computer screen; (b) generating the spacial structure of a compound to be tested; and (c) testing to determine if the compound interacts with said IgE binding domain, wherein such an interaction indicates that the compound is capable of inhibiting the binding of an IgE antibody to a FcεRIα protein. In a preferred embodiment, step (a) includes the step of identifying one or more amino acid(s) in the IgE binding domain of the model that interact directly with the Fc domain of an IgE antibody when the Fc domain binds to the IgE binding domain. Preferably a compound to be tested will interact directly with one 20 or more of those amino acid(s). Preferred amino acids with which an inhibitory compound should interact are disclosed herein.

The present invention also includes inhibitory compounds isolated in accordance with the methods disclosed herein. Methods to produce such compounds in quantities sufficient for use, for example, as protective agents (e.g., preventatives or therapeutics) are known to those skilled in the art. It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of any suitable FcRs (i.e., model modifications) and to identify compounds that inhibit the binding of antibodies to such FcRs.

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The present invention also includes use of a 3-D model of the present invention to rationally design and construct modified forms of FcRs that have one or more improved functions, such as, but not limited to, increased activity, increased stability and increased solubility compared to an unmodified FcR. Muteins of the present invention include full-length proteins as well as fragments (i.e., truncated versions) of such proteins.

One embodiment of the present invention is a FcR that comprises a mutein that binds to a Fc domain of an antibody. Such a mutein has an improved function compared to a protein comprising SEQ ID NO:2 or SEQ ID NO:4. Examples of such an improved function include, but are not limited to, increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility. Such a mutein can be produced by a method that includes the steps of: (a) analyzing a 3-D model substantially representing the atomic coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8 to identify at least one amino acid of the protein represented by the model which if replaced by a specified amino acid would effect the improved function of the protein; and (b) replacing the identified amino acid(s) to produce a mutein having the improved function. Knowledge of the coordinates allows one to target specific residues, e.g. in the hydrophobic core or on the surface, to generate an accessible set of variants that can then be selected for a particular property, e.g. high stability, high affinity, altered substrate specificity, or other desirable properties (i.e., improved functions). Without the coordinates, one would have to analyze an 20 extraordinarily large number of variants, e.g., on the order of ~1011 possibilities. The structure, in contrast, allows one to pick the most relevant residues for selecting a desired property by, for example, phage display or other methods. In a preferred embodiment, replacement of one or more amino acids does not substantially disrupt the 3-D structure of the protein; i.e., the modified protein, or mutein, is still capable of binding to the Fc domain of an antibody. A preferred mutein is a FcR that binds to a Fc domain of an IgE antibody, although the invention also covers muteins binding to other classes of antibodies.

In one embodiment, a mutein of the present invention has increased stability compared to its unmodified counterpart. As used herein, increased stability refers to the

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ability of a mutein to be more resistant, for example, to higher or lower temperature, to more acidic or basic pH, to higher or lower salt concentrations, to oxidation and/or reduction, to deamidation, to other forms of chemical degradation and to proteolytic degradation compared to unmodified FcR. Increased stability can also refer to the ability of a mutein of the present invention to be stable for a longer period of time either during storage (i.e., to have a longer shelf life) or during use (i.e., to have a longer half-life under reaction conditions) than does an unmodified protein. Muteins of the present invention can also exhibit a decreased entropy of unfolding, thereby stabilizing the proteins. Increased stability can be measured using a variety of methods known to those skilled in the art; examples include, but are not limited to, determination of melting temperature, thermal denaturation, pressure denaturation, enthalpy of unfolding, free 10 energy of the protein, or stability in the presence of a chaotropic agents such as urea, guanidinium chloride, guanidinium thiocyanate, etc. A preferred mutein of the present invention has a melting temperature substantially higher than that of an unmodified FcR. Preferably the melting temperature of a mutein is at least about 1°C higher, and more preferably at least about 10°C higher than the melting temperature of the corresponding unmodified protein. Also preferred is a mutein having binding activity over a pH range that is at least about 1 pH unit higher and/or lower than the active pH range of the corresponding unmodified protein.

Another embodiment of the present invention is a mutein that exhibits increased affinity for a Fc domain of an antibody compared to its unmodified counterpart. As used herein, a mutein having increased affinity is a FcR that exhibits a higher affinity constant (K_A) or lower dissociation co_{in} tant (K_D) than its unmodified counterpart. Such a higher affinity constant can be achieved by increasing the association rate (k_A) between the mutein and the Fc domain and/or decreasing the dissociation rate (k_A) between the mutein and the Fc domain. A preferred mutein of the present invention has a K_A for a Fc domain of at least about 3 x 10° liters/mole (M^{-1}) , which is equivalent to a K_D of less than or equal to about 3.3 x 10° moles/liter (M). More preferred is a mutein having a K_A for a Fc domain of at least about 2 x 10° M^{-1} , and even more preferably of at least about 1 x 10° liters/mole-second as well as a mutein having a k_A for a Fc domain of less about 1 x 10° liters/mole-second as well as a mutein having a k_A for a Fc domain of less

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than or equal to 3 x 10⁻⁵/second. More preferred is a mutein having a k_a for a Fc domain of at least about 3 x 10⁵ liters/mole-second, and even more preferably of 1 x 10⁶ liters/mole-second. Also preferred are muteins having a k_d for a Fc domain of less than or equal to 1 x 10⁻⁵/second or even more preferably less than or equal to 3 x 10⁻⁴/second. A preferred Fc domain is that of an IgE antibody. Methods to measure such binding constants is well known to those skilled in the art; see, for example, Cook et al., 1997, *ibid.*, which reports the following values for the binding of human FceRIα protein to human IgE: k_{a1} of 3.5 (±0.9) x 10⁵ M⁻¹s⁻¹; k_{a2} of 8.6 (±3.5) x 10⁴ M⁻¹s⁻¹; k_{d1} of 1.2 (±0.1) x 10⁻² s⁻¹; k_{d2} of 3.2 (±0.8) X 10⁻⁵ s⁻¹; K_{A1} of 2.0 X10⁷ M⁻¹; K_{A2} of 2.9 X10⁹ M⁻¹.

Another embodiment of the present invention is a mutein that exhibits altered substrate specificity compared to its unmodified counterpart. A mutein exhibiting altered substrate specificity is a mutein that binds with increased affinity to a Fc domain of an antibody class or antibody species of a different type than that normally bound by its unmodified counterpart. In one embodiment, a mutein of a human FceRIa protein with altered substrate specificity is a FcR that binds with increased affinity to a IgE antibody of another mammal, such as, but not limited to, a canine, feline, equine, murine, or rat IgE antibody. In another embodiment, a mutein of a human FceRIa protein with altered substrate specificity is a FcR that binds with increased affinity to an antibody of another class, such as IgG, IgM, IgA, or IgD, with IgG being preferred.

Such a mutein can also show altered species substrate specificity. Methods to determine whether a mutein exhibits altered substrate specificity are well known to those skilled in

Yet another embodiment of the present invention is a mutein that exhibits increased solubility compared to its unmodified counterpart. Such a protein is less likely to form aggregates. Methods to determine whether a mutein exhibits increased solubility are well known to those skilled in the art.

As disclosed herein, the 3-D model representing a FceRI α protein is advantageous in determining strategies for producing muteins having an improved function, e.g., for identifying targets to modify in order to obtain muteins having improved functions. Examples of targets are as follows. A key feature of the human FceRI α_{1-176} protein or the FceRI α_{1-172} protein is the crystal contacts in five space groups,

a subset of which are predicted to interact directly with a Fc domain of an IgE antibody. Such contacts are included in the IgE binding domain which is unique for human FceRIa in that the domain includes a tryptophan-containing hydrophobic ridge positioned on the top face of the crystal structure (i.e., amino acids W87, W110, W113, and W156 of SEQ ID NO:2 or SEQ ID NO:4) and an FG loop comprising amino acids from 155 to 158 of SEQ ID NO:2 or SEQ ID NO:4 that protrudes above the interface in an unusual manner. Another key feature is the interface between domain 1 and domain 2 (i.e., the D1D2 interface) which includes amino acids 12, 13, 14, 15, 16, 17, 18, 20, 84, 85 and 86 in D1 and 87, 88, 89, 90, 91, 92, 93, 95, 104, 106, 108, 110, 111, 161, 163, 164, and 165 in D2 of SEQ ID NO:2 or SEQ ID NO:4. Also important are the two domains themselves: D1 includes amino acids 1 through 86 of SEQ ID NO:2 or SEQ ID NO:4; and D2 includes amino acids 87 through 176 of SEQ ID NO:2 or amino acids 87 through 172 of SEQ ID NO:4. Another important feature is the cleft between D1 and D2, which can be identified using the coordinates. Other areas of interest include the hydrophobic core which can be identified using the coordinates, the A'B loop of D1, which includes 15 amino acids 18 and 19, the EF loop of D1, which includes amino acids 59-63, the BC loop of D2, which includes amino acids 110-114, the C strand of D2, which includes amino acids 114-123, the CC' loop of D2, which includes amino acids 123-125, the C'E loop of D2, which includes amino acids 127-134, in the different confirmations observed in the five crystal forms, and the F strand of D2, which includes amino acids 147-155 of SEQ ID NO:2 or SEQ ID NO:4. Yet another striking feature is the finding that the amino and carboxyi termini of the human $FceRIa_{1-176}$ protein are only 10 angstroms apart.

In accordance with the present invention, a mutein having an improved function can be produced by a method that includes replacing at least one amino acid based on 25 information derived from analyzing a 3-D model of the present invention to produce the mutein having the improved function. Knowledge of the structure of the extracellular domain of a human FceRIa protein crystal, for example, permits the rational design and construction of modified forms of the protein by permitting the prediction and production of substitutions, insertions, deletions, inversions and/or derivatizations that effect an improved function. That is, analysis of 3-D models of the present invention

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provide information as to which amino acid residues are important and, as such, which amino acids can be changed without harming the protein. In making amino acid replacements, it is preferred to use amino acid replacements that have similar numbers of atoms and that allow conservation of salt bridges, hydrophobic interactions and 5 hydrogen bonds unless the goal is to purposefully change such interactions. The 3-D structure of the human FceRIa protein suggests that large deletions may not be desirable, particularly due to the relation between the various domains of the protein and the observation that most of the structure is well ordered in the crystal. An exception to this is the non-constrained loops of D1, which apparently could be deleted or shortened without harming the protein's function. These loops span amino acids 31-35 and 70-74 of SEQ ID NO:2 or SEQ ID NO:4.

It is to be appreciated that although one amino acid replacement capable of improving the function of a protein can substantially improve that function, more than one amino acid replacement can result in cumulative changes depending on the number and location of the replacements. For example, although one amino acid replacement capable of substantially increasing the stability of a protein can increase the melting temperature of that modified protein by about 1°C, about 5 to about 6 replacements may increase the melting temperature of the resultant protein by about 10°C.

In accordance with the present invention, the 3-D model of the human FceRIa protein has been analyzed, using techniques known to those skilled in the art, to determine the accessibility of the amino acids represented within the model to solvert. Such information is provided in, for example, Table 2, Table 9, Table 10, Table 11, and Table 12.

A number of methods can be used to produce muteins of the present invention. One method includes the steps of: (a) analyzing a 3-D model substantially representing the coordinates specified in Table 1, Table 5, Table 6, Table 7, or Table 8 to identify at least one amino acid of the modeled protein which if replaced by a specified amino acid would effect an improved function; and (b) replacing the identified amino acid(s) to produce a mutein having that improved function. In one embodiment, a method to produce a mutein includes the steps of (a) comparing a key region of a model of a human 30 FcεRIα protein with the amino acid sequence of a FcR having an improved function

compared to the unmodified FceRIa protein in order to identify at least one amino acid segment of the FcR with the improved function that if incorporated into the FccRI α protein represented by the model would give the FceRIa protein the improved function; and (b) incorporating the segment into the FceRIa protein, thereby providing a mutein with the improved function. In another embodiment, a method to produce a protein includes the steps of: (a) using a model representing a human FceRIa protein to identify a 3-D arrangement of residues that can be randomized by mutagenesis to allow the construction of a library of molecules from which a improved function can be selected; and (b) identifying at least one member of the mutagenized library having the improved function. In one example, a mutein is produced by a method that includes the steps of: (a) effecting random mutagenesis of nucleic acid molecules encoding a target of a 10 FCERIa protein as identified by analyzing a model of that protein, such as an IgE binding domain; (b) cloning such mutagenized nucleic acid molecules into a phage display library, wherein said phage display library expresses the target; and (c) identifying at least one member of the library that expresses a target with an improved function, such as an antibody binding domain exhibiting increased affinity for an antibody. As stated 15 above, the model allows the use of this technique in a straightforward manner that could not be accomplished in the absence of the model. It is to be also noted that these methods can also be used with other models of the present invention to produce muteins of the present invention. 20

The present invention includes a number of methods, based on analysis of a 3-D model of the present invention, to replace (i.e., add, delete, substitute, invert, derivatize) at least one amino acid residue in the protein represented by the model in order to produce a mutein of the present invention. Such methods include, but are not limited to:

25 (a) replacing at least one amino acid in at least one non-constrained loop of domain 1 in an area proximal to the FceRI gamma chain putative binding site; (b) joining an amino-terminal amino acid residue to a carboxyl-terminal amino acid residue of an extracellular domain of a FceRIα protein; (c) replacing at least one amino acid site with an amino acid suitable for derivatization; (d) replacing at least one pair of amino acids of the protein with a cysteine pair to enable the formation of a disulfide bond that stabilizes the protein; (e) removing at least a portion of the region between the B strand and C strand

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of domain 1; (f) removing at least a portion of the region between the C strand and E strand of domain 1; (g) replacing at least one amino acid in the IgE binding domain in order to increase the affinity between an IgE antibody and the protein; (h) replacing at least one amino acid of the protein with an amino acid such that the replacement decreases the entropy of unfolding of the protein; (i) replacing at least one asparagine or glutamine of the protein with an amino acid that is less susceptible to deamidation than is the amino acid to be replaced; (j) replacing at least one methionine, histidine or tryptophan with an amino acid that is less susceptible to an oxidation or reduction reaction than is the amino acid to be replaced; (k) replacing at least one arginine of the protein with an amino acid that is less susceptible to dicarbonyl compound modification than is the amino acid to be replaced; (1) replacing at least one amino acid of the protein susceptible to reaction with a reducing sugar sufficient to reduce protein function with an amino acid less susceptible to that reaction; (m) replacing at least one amino acid of the protein with an amino acid capable of increasing the stability of the inner core of the protein; (n) replacing at least one amino acid of the protein with at least one N-linked glycosylation site; (o) replacing at least one N-linked glycosylation site of the protein 15 with at least one amino acid that does not comprise an N-linked glycosylation site; and (p) replacing at least one amino acid of the protein with an amino acid that reduces aggregation of the protein.

Amino acid replacements can be carried out using recombinant DNA techniques known to those skilled in the art, including site-directed mutagenesis (e.g., oligonucleotide mutagenesis, random mutagenesis, polymerase chain reaction (PCR)-aided mutagenesis, gapped-circle site-duected mutagenesis) or chemical synthetic methods of a nucleic acid molecule encoding the desired protein, such as, but not limited to a human FceRIa protein, followed by expression of the mutated gene in a suitable expression system, preferably an insect, mammalian, bacterial, yeast, insect, or mammalian expression system. See, for example, Sambrook et al., *ibid*.

One embodiment of the present invention is a mutein in which at least one amino acid in at least one non-constrained loop of a FceRI α protein is replaced in order to improve a function of the protein. Finding that the human FceRI α protein had such loops was surprising, and it is believed, without being bound by theory, that a mutein in

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which at least a portion of at least one such loop is replaced, would at least exhibit enhanced stability. In a preferred embodiment, at least a portion of one or more of such loops is (are) deleted. Preferred loops to replace are in domain 1 (i.e., spanning amino acids 31-35 and 70-74 of SEQ ID NO:2 or SEQ ID NO:4), preferably in an area proximal to the FceRI gamma chain putative binding site, i.e., the site on the FcεRIα protein to which the gamma chain of the high affinity Fc epsilon receptor is thought to bind. In a preferred embodiment, one or more amino acids is replaced to make loops shorter, but including 1 or 2 hydrophobic residues to pack toward the protein interior and at least one hydrophilic residue to maintain solubility.

Another embodiment of the present invention is a mutein of the extracellular domain of a FceRIa protein in which an N-terminal (amino-terminal) amino acid residue is joined, preferably covalently, to a C-terminal (carboxyl-terminal) amino acid residue in order to improve a function of the protein. Finding that the N-termini and C-termini of the human FceRIa protein were only 10 angstroms apart was quite surprising. Without being bound by theory, it is believed that such a mutein would at least exhibit enhanced stability. Furthermore, a covalent linker used to join the termini could also include a substance useful, for example, to anchor a mutein on a surface, as would be useful, for example, in a diagnostic assay, or to label the mutein. For a protein consisting of SEQ ID NO:2, a preferred N-terminal residue is an amino acid residue at position 1, 2, or 3 of SEQ ID NO:2, and a preferred C-terminal residue is an amino acid 20 residue at position 174, 175, or 176 of SEQ ID NO:2. Covalent linkage can be accomplished by methods known to those skilled in the art, such as, but not limited to, adding one or more N-terminal and C-terminal cysteines and crosslinking them with chemical compounds, adding additional residues in the coding sequence to allow the formation of a disulfide bond, or adding one or more lysines and coupling them through 25 a 10 angstrom linker, and including non-natural amino acid analogues by synthetic methods or by a combination of biosynthetic and organosynthetic methods. Examples of a substance to add to a covalent linker includes: ligands useful in allowing for the attachment of a mutein to a surface, such as biotin and related compounds, avidin and related compounds, metal binding compounds, sugar binding compounds, 30 immunoglobulin binding domains, and other tag domains; and detectable markers, such

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as enzyme labels, physical labels, radioactive labels, fluorescent labels, chemiluminescent labels, and chromophoric labels. Examples include, but are not limited to, alkaline phosphatase, horseradish peroxidase, digoxygenin, luciferase, other light-generating enzymes and magnetic beads. It is also to be noted that ligands can function as detectable markers.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid suitable for derivatization. Muteins in which at least one amino acid is replaced with an amino acid suitable for derivatization include proteins that are chemically modified (e.g., a lysine already existing on the protein is modified) as well as those in which an amino acid residue is replaced with a different amino acid residue (e.g., a glycine with a lysine) as well as proteins to which a substance is added, preferably to the amino or carboxyl terminus of the protein. Examples of such substances include ligands and detectable markers as disclosed above. Preferable amino acids to replace include residues that are solvent exposed (e.g., those listed in Table 2, Table 9, Table 10, Table 11, or Table 12), but that are preferably not within about 10 angstroms of the IgE binding domain. In one embodiment, a glycosylation site, or other solvent exposed site, is replaced with a charged or polar residue to increase solubility or create more stable muteins. Glycosylation sites in human FceRIa protein include amino acids 21, 42, 50 74, 135, 140, and 166 of SEQ ID NO:2 or SEQ ID NO:4. A preferred amino acid to use as a replacement, or to chemically modify directly, includes a cysteine 20 or a lysine, with a cysteine being preferred. Compounds to use in chemical derivatizations are known to those skilled in the art; cysteines can, for example, be derivatized with maleimides.

Another embodiment of the present invention is a mutein in which a pair of amino acids have been replaced with a cysteine pair in order to improve the function of 25 the mutein, at least by increasing stability. Cysteine pairs can be substituted into a FcεRIα protein at any two residue positions identified with available programs and algorithms that would allow the formation of an undistorted disulfide bridge. In one embodiment, a serine and lysine near the termini of the protein is each replaced with a cysteine. In another embodiment, cysteine pairs are replaced with other amino acids, 30 such as serines to eliminate non-essential disulfide bonds.

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Another embodiment of the present invention is a mutein in which at least one amino acid is replaced in the region between the B strand and C strand of domain 1 and/or the region between the C and E strand of domain 1. In a preferred embodiment, at least a portion of such a region is deleted.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced in the IgE binding domain in order to increase the affinity between an IgE antibody and the protein. Preferred residues to replace are in or near the IgE binding domain, or IgE binding site, as determined by analysis of the 3-D model. Such residues are preferably within about 10 angstroms of residues identified by mutagenesis and further shown by model to be in an IgE binding site. Examples of such residues include amino acids 87, 110, 113, 115, 117, 118, 120, 121, 122, 123, 128, 129, 131, 149, 153, 154, 155, 156, 157, 158, and 159 of SEQ ID NO:2 or SEQ ID NO:4, and amino acids within 10 angstroms of such listed amino acids. In one embodiment, preferred amino acids to replace include amino acids 87, 115, 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of any of the listed amino acids, with amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 as well as any surface residue within about 10 angstroms of amino acids 87, 117, 121, 123, 128, 159 of SEQ ID NO:2 or SEQ ID NO:4 being particularly preferred. It is to be noted that amino acids 115, 118, 120, 131, 149 and 155 of SEQ ID NO:2 or SEQ ID NO:4 are buried, and 20 that amino acids that are partially buried or glycine include residues 122, 129 and 153. Additional amino acid residues to target include those in the A'B loop of D1, and EF loop of D1. Note that these residues are not the same as those shown in mutation studies to affect IgE binding since some of those mutants have mutations in amino acids that are internal to the protein; this finding can only be made by analysis of a model of the 25 present invention.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid capable of increasing the stability of the inner core or surface of the protein. Preferred amino acids to replace are hydrophilic residues located in the hydrophobic core of the protein and/or hydrophobic amino acids at the protein surface that are not within about 10 angstroms of the IgE binding domain

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residues of D1 or D2. Preferred amino acids to replace into the hydrophobic core are hydrophobic residues such as, but not limited to, tryptophan, leucine, isoleucine, valine and alanine, as well as space filling amino acids, such as other aromatic amino acids. Preferred amino acids to replace onto the surface are polar amino acids, such as, but not limited to, glutamic acid, glutamine, aspartic acid, asparagine, histidine and serine. Muteins having one or more such amino acid replacements would exhibit at least increased stability and/or reduced aggregation. Additional preferred amino acid replacements are those that introduce salt bridges at the protein surface to stabilize protein folds. It is noted that the cysteines at positions 26 and 68 of SEQ ID NO:2 or SEQ ID NO:4 form a disulfide bond in domain 1 that is somewhat exposed to solvent, depending especially on the conformation of the D1 "30 loop" (i.e., amino acids 31-35 of SEQ ID NO:2 or SEQ ID NO:4). In one embodiment, changes in neighboring residues can be made in, for example, residues 1-5, 27-37, 49-52, or 69-75, to bury this disulfide from exposure to solvent. For example, phage display of receptors with randomized mutations in the 30 loop, might be useful for selecting receptors that react 15 less well with reducing reagents and have a more stable D1 core.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid that decreases the entropy of unfolding of the protein. The entropy of unfolding of a protein can be measured and compared to that of another protein using techniques known to those skilled in the art. A number of methods known to those skilled in the art can be used to reduce the number of protein conformations possible in the unfolded state, thereby improving the ability of the protein to fold correctly. One embodiment of the present invention for decreasing the entropy of unfolding includes replacing at least one amino acid of the protein with a specified amino acid in order to maintain certain desirable phi and psi backbone conformation angles in the protein; see, for example, PCT International Publication No. WO 89/01520, by Drummond et al., published February 23, 1989. For example, a proline residue in a protein constrains the backbone conformation to certain restricted angles. Analysis of a 3-D model of a protein of the present invention permits the identification of candidate replacement positions in the protein that have the conformation expected for a proline, but that do not have a proline in them. Such knowledge is used to

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introduce prolines into such candidate replacement positions to "anchor" the resultant mutein in the desired conformation. The 3-D model also permits the identification of candidate replacement sites that if replaced with a proline do not substantially disrupt the 3-D structure of the resultant protein. Similarly, glycines in appropriate positions can be replaced with an amino acid having a β carbon atom or a branched β carbon atom, preferably an alanine, in order to stabilize the backbone of the protein.

Another embodiment of the present invention is a mutein in which at least one asparagine or glutamine is replaced with an amino acid that is less susceptible to deamidation. Preferred amino acids to replace include solvent accessible asparagines and glutamines.

Another embodiment of the present invention is a mutein in which at least one methionine, histidine or tryptophan is replaced with an amino acid that is less susceptible to an oxidation or reduction reaction. Preferred amino acids to replace include M98, H70, and H41. It would not be preferred to replace any of the tryptophans, nor H108 or H134 of SEQ ID NO:2 or SEQ ID NO:4.

Another embodiment of the present invention is a mutein in which at least one arginine is replaced with an amino acid that is less susceptible to dicarbonyl compound modification. Although R174 could be changed, it would probably not be preferable to change amino acids at the D1D2 interface or near the IgE binding site, such as amino acids 15, 106, or 111 of SEQ ID NO:2.

Another embodiment of the present invention is a mutein in which at least one amino acid that is susceptible to reaction with a reducing sugar sufficient to reduce protein function is replaced with an amino acid that is less susceptible to such a reaction. For example, lysines, glutamines and asparagines that could react with a sugar, such as galactose, glucose or lactose can be replaced with non-reactive amino acids.

Another embodiment of the present invention is a mutein in which one or more N-linked glycosylation sites are added to or removed from the protein, preferably by substitution with an appropriate amino acid. A FceRIa protein with additional N-linked glycosylation sites is more soluble. The ability to design a FceRIa protein having fewer, or no, N-linked glycosylation sites is also valuable as production of such a protein from production run to production run is likely to be more uniform. One embodiment is a

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FceRIα mutein with no N-linked glycosylation sites that is stable, active, and soluble. Such a protein has an advantage of being produced in *E*. coli at low cost. In one embodiment, one or more exposed hydrophobic amino acids are changed to charged residues that form salt bridges to stabilize the protein fold and make it soluble. It is to be noted that the glycosylation sites that appear to be most often observed in the different crystal structures in the same conformation are the carbohydrate attached to positions 42 and 166 of SEQ ID NO:2 or SEQ ID NO:4. The carbohydrate attached to position 42 always appears to cover the phenylalanine at position 60 of SEQ ID NO:2 or SEQ ID NO:4. As such, one embodiment of the present invention is to remove the glycosylation site at position 42, e.g., by substitution with a suitable amino acid. This embodiment has the additional advantage that the resultant mutein has an exposed phenylalanine at position 60, thereby leading to increased IgE binding activity.

Another embodiment of the present invention is a mutein in which at least one amino acid is replaced with an amino acid that reduces aggregation and increases solubility of the protein, such as, for example, replacing one or more hydrophobic residues on the surface with one or more hydrophilic residues. Other examples of such amino acids to replace are disclosed herein.

Another embodiment of the present invention to enhance stability is the addition of polyethylene glycol (PEG) groups to a FcR protein, i.e., to produce a "pegylated" FcR protein. In one embodiment, the PEG group(s) can substitute for carbohydrate group(s) due to removal of one or more N-glycosylation sites. Such PEG group(s) can be attached to easily modifiable residues, such as cysteines or lysines, on the surface of the protein, such residues identifiable by analysis of a 3-D model of the present invention.

Another embodiment of the present invention is a mutein that comprises a FcR having a substance, such as a ligand or detectable marker, attached to an amino acid of the protein such that the substance does not substantially interfere with the antibody binding activity of the protein. The substance is attached in such a manner that the substance is also capable of performing its function, such as binding to a second member of a ligand pair or enabling detection of the protein. The FcR to which a substance is attached can be either an unmodified protein or a mutein of the present invention. Suitable attachment sites can be identified using 3-D models of the present invention.

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Preferred attachment sites include solvent exposed amino acids, such as those listed in Table 2, Table 9, Table 10, Table 11, or Table 12. Substances can be attached, or conjugated, to the protein using techniques known to those skilled in the art. It is to be appreciated that a preferred method to attach a substance to an amino acid is to modify that amino acid to have a reactive attachment site, such as is present on cysteine and lysine amino acids. As such, an attachment site comprising a solvent exposed amino acid refers to the nature of the amino acid prior to any modification required for attachment. Examples of suitable substances to attach to a FcI include any compound capable of binding to or reacting with another substance, such as those described for attachment to a covalent linker.

It is to be appreciated that muteins of the present invention can include amino acids which are not modified because they would negatively impact the function of the protein. Such amino acids can be identified using a 3-D model of the present invention.

It should also be appreciated that it is within the scope of the present invention to expand the use of models of the present invention to produce models of and make modifications to any suitable FcRs or other Ig domain-containing proteins to produce muteins having a desired function.

The present invention also includes nucleic acid molecules that encode muteins of the present invention as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Methods to produce such proteins are also disclosed herein.

The present invention includes an isolated FcεRIα protein that consists of SEQ ID NO:2, i.e., PhFcεRIα₁₋₁₇₆. Also included in the present invention is a protein consisting of an extracellular domain of a FcεRIα protein that is structurally homologous to an isolated FcεRIα protein consisting of SEQ ID NO:2. As used herein, a protein that is structurally homologous to PhFcεRIα₁₋₁₇₆ is a protein that (a) includes both D¹ and D2 domains, (b) shares at least about 30%, and preferably at least about 40%, amino acid sequence identity with SEQ ID NO:2, as determined using a ALIGN with default parameters, optimal global alignment of two sequences with no short-cuts, (c) displays a substantially equivalent affinity for an IgE antibody as does a complete extracellular domain of the corresponding FcεRIα protein, and (d) produces crystals having sufficient

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quality to enable structure determination. Examples of such proteins include a human FceRIα protein having SEQ ID NO:4, i.e., PhFceRIα₁₋₁₇₂ and a human FceRIα protein having an amino acid sequence that spans from amino acid 3 through amino acid 174 of SEQ ID NO:2, i.e., PhFc ϵ RI α_{3-174} . It is to be noted that these examples are provided to 5 clarify the definition of a structurally homologous FcεRIα protein and are not intended to limit the scope of such proteins. That is, a Fc ϵ RI α protein that is structurally homologous to PhFceRI α_{1-176} is any mammalian FceRI α protein having the listed characteristics. Preferred are human, canine, feline, equine, murine and rat proteins that are structurally homologous to PhFceRI α_{1-176} . Also included herein are nucleic acid molecules to encode such proteins as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Methods to produce such proteins are also disclosed herein. Preferably such proteins are produced in insect cells.

The present invention also includes a FceRIa protein consisting of SEQ ID NO:4 except that the isoleucine at position 170 has been replaced by a cysteine. Also included in the present invention is a protein consisting of an extracellular domain of a $FceRI\alpha$ protein that is structurally homologous to an isolated FceRIa protein consisting of SEQ ID NO:4 except that the isoleucine at position 170 has been replaced by a cysteine.

The present invention also includes the following novel structures as identified by a 3-D model of the present invention: a crystal contact cluster, preferably involved in IgE binding; a tryptophan-containing hydrophobic ridge; a FG loop in D2; a D1D2 interface; a cleft between D1 and D2; a domain 1; a domain 2; a hydrophobic core; a 20 A'B loop of D1; a EF loop of D1; a BC loop of D2; a C strand of D2; a CC' loop of D2; a C'E loop of D2; and a strand of D2. Also included herein are nucleic acid molecules to encode such structures as well as recombinant molecules and recombinant cells that include such nucleic acid molecules. Also included are methods to produce such structures and models thereof.

The present invention also includes isolated nucleic acid molecules encoding proteins of the present invention, including, but not limited to, proteins comprising unmodified extracellular domains of FcRs, novel structures within such proteins, and muteins. As used herein, an isolated nucleic acid molecule encoding a protein is a nucleic acid molecule that has been removed from its natural milieu. As such, "isolated"

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does not reflect the extent to which the nucleic acid molecule has been purified. An isolated nucleic acid molecule can be DNA, RNA, or derivatives of either DNA or RNA.

A nucleic acid molecule encoding a mutein of the present invention can be produced by mutation of parental protein genes (e.g., unmodified or previously modified protein-encoding genes, or portions thereof) using recombinant DNA techniques heretofore disclosed or by chemical synthesis. Resultant mutein nucleic acid molecules can be amplified using recombinant DNA techniques known to those skilled in the art, such as PCR amplification or cloning (see, for example, Sambrook et al., ibid.), or by chemical synthesis. A mutein can also be produced by chemical modification of a protein expressed by a nucleic acid molecule encoding an unmodified protein or muteinencoding gene.

Proteins of the present invention can be produced in a variety of ways, including production and recovery of recombinant proteins and chemical synthesis. In one embodiment, a protein of the present invention is produced by culturing a cell capable of expressing the protein under conditions effective to produce the protein, and recovering the protein. A preferred cell to culture is a recombinant cell that is capable of expressing the protein, the recombinant cell being produced by transforming a host cell with one or more nucleic acid molecules of the present invention. Transformation of a nucleic acid molecule into a host cell can be accomplished by any method by which a nucleic acid molecule can be inserted into a cell. Transformation techniques include, but are not limited to, transfection, electroporation, microinjection, lipofection, adsorption, and protoplast fusion. A recombinant cell may remain unicellular or may grow into a tissue, organ or a multicellular organism. Transformed nucleic acid molecules of the present invention can remain extrachromosomal or can integrate into one or more sites within a chromosome of a host cell in such a manner that their ability to be expressed is retained. 25

Suitable host cells to transform include any cell that can be transformed. Host cells can be either untransformed cells or cells that are already transformed with at least one nucleic acid molecule. Host cells of the present invention can be endogenously (i.e., naturally) capable of producing a protein of the present invention, but such cells are not preferred. Host cells of the present invention can be any cell that when transformed with a nucleic acid molecule of the present invention are capable of producing a protein of the

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present invention, including bacterial, yeast, other fungal, insect, animal, and plant cells. Preferred host cells include bacterial, yeast, insect and mammalian cells, and more preferred host cells include Escherichia, Bacillus, Saccharomyces, Pichia, Trichoplusia, Spodoptera and mammalian cells. Particularly preferred host cells are Trichoplusia ni cells, Spodoptera frugiperda cells, and Chinese hamster ovary cells.

A recombinant cell is preferably produced by transforming a host cell with a recombinant molecule comprising a nucleic acid molecule of the present invention operatively linked to an expression vector containing one or more transcription control sequences. The phrase operatively linked refers to insertion of a nucleic acid molecule into an expression vector in a manner such that the molecule is able to be expressed when transformed into a host cell. As used herein, an expression vector is a DNA or RNA vector that is capable of transforming a host cell, of replicating within the host cell, and of effecting expression of a specified nucleic acid molecule. Expression vectors can be either prokaryotic or eukaryotic, and are typically viruses or plasmids. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including in bacterial, yeast, 15 other fungal, insect, animal, and plant cells. Preferred expression vectors of the present invention can direct gene expression in bacterial, yeast, insect and mammalian cells.

Nucleic acid molecules of the present invention can be operatively linked to expression vectors containing regulatory control sequences such as promoters, operators, repressors, enhancers, termination sequences, origins of replication, and other regulatory control sequences that are compatible with the host cell and that control the expression of the nucleic acid molecules. In particular, recombinant molecules of the present invention include transcription control sequences. Transcription control sequences are sequences which control the initiation, elongation, and termination of transcription. Particularly important transcription control sequences are those which control 25 transcription initiation, such as promoter, enhancer, operator and repressor sequences. Suitable transcription control sequences include any transcription control sequence that can function in at least one of the recombinant cells of the present invention. A variety of such transcription control sequences are known to those skilled in the art. Preferred 30

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transcription control sequences include those which function in bacterial, yeast, insect and mammalian cells.

It may be appreciated by one skilled in the art that use of recombinant DNA technologies can improve expression of transformed nucleic acid molecules by manipulating, for example, the number of copies of the nucleic acid molecules within a host cell, the efficiency with which those nucleic acid molecules are transcribed, the efficiency with which the resultant transcripts are translated, and the efficiency of posttranslational modifications. Recombinant techniques useful for increasing the expression of nucleic acid molecules of the present invention include, but are not limited to, operatively linking nucleic acid molecules to high-copy number plasmids, integration of the nucleic acid molecules into one or more host cell chromosomes, addition of vector 10 stability sequences to plasmids, substitutions or modifications of transcription control signals (e.g., promoters, operators, enhancers), substitutions or modifications of translational control signals (e.g., ribosome binding sites, Shine-Dalgarno sequences), modification of nucleic acid molecules of the present invention to correspond to the codon usage of the host cell, deletion of sequences that destabilize transcripts, and use of 15 control signals that temporally separate recombinant cell growth from recombinant protein production during fermentation. The activity of an expressed recombinant protein of the present invention may be improved by fragmenting, modifying, or derivatizing nucleic acid molecules encoding such a protein. 20

In accordance with the present invention, recombinant cells can be used to produce proteins by culturing such cells under conditions effective to produce such a protein, and recovering the protein. Lefective conditions to produce a protein include, but are not limited to, appropriate media, bioreactor, temperature, pH and oxygen conditions that permit protein production. An appropriate medium refers to any medium in which a cell of the present invention, when cultured, is capable of producing the protein. An effective medium is typically an aqueous medium comprising assimilable carbohydrate, nitrogen and phosphate sources, as well as appropriate salts, minerals, metals and other nutrients, such as vitamins. The medium may comprise complex nutrients or may be a defined minimal medium. Cells of the present invention can be cultured in conventional fermentation bioreactors, which include, but are not limited to, 30

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batch, fed-batch, cell recycle, and continuous fermentors. Culturing can also be conducted in shake flasks, test tubes, microtiter dishes, and petri plates. Culturing is carried out at a temperature, pH and oxygen content appropriate for the recombinant cell. Such culturing conditions are well within the expertise of one of ordinary skill in the art.

Depending on the vector and host system used for production, resultant proteins may either remain within the recombinant cell; be secreted into the fermentation medium; be secreted into a space between two cellular membranes, such as the periplasmic space in E. coli; or be retained on the outer surface of a cell or viral membrane. The phrase "recovering the protein" refers simply to collecting the whole fermentation medium containing the protein and need not imply additional steps of separation or purification. Proteins of the present invention can be purified using a variety of standard protein purification techniques, such as, but not limited to, affinity chromatography, ion exchange chromatography, filtration, electrophoresis, hydrophobic interaction chromatography, gel filtration chromatography, reverse phase chromatography, chromatofocusing and differential solubilization. 15

The present invention also includes isolated (i.e., removed from their natural milieu) antibodies that selectively bind to a FcR of the present invention (i.e., anti-FcR antibodies). As used herein, the term "selectively binds to" FcR refers to the ability of antibodies of the present invention to preferentially bind to specified proteins of the present invention. Binding can be measured using a variety of methods standard in the art including enzyme immunoassays (e.g., ELISA), immunoblot assays, etc.; see, for example, Sambrook et al., ibid. Isolated antibodies of the present invention can include antibodies in a bodily fluid (such as, but not limited to, serum), or antibodies that have been purified to varying degrees. Antibodies of the present invention can be polyclonal or monoclonal. Functional equivalents of such antibodies, such as antibody fragments and genetically-engineered antibodies (including single chain antibodies or chimeric antibodies that can bind to more than one epitope) are also included in the present invention. Antibodies can be produced using methods known to those skilled in the art. A preferred method to produce antibodies of the present invention includes (a) administering to an animal an effective amount of a protein of the present invention to produce the antibodies and (b) recovering the antibodies. In another method, 30

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antibodies of the present invention are produced recombinantly using techniques as heretofore disclosed to produce proteins of the present invention. Antibodies raised against defined proteins can be advantageous because such antibodies are not substantially contaminated with antibodies against other substances that might otherwise cause interference in a diagnostic assay or side effects if used in a therapeutic composition.

Antibodies of the present invention have a variety of potential uses that are within the scope of the present invention. Examples of such uses are disclosed in WO 98/27208, *ibid.*, see, for example, page 24.

A FcR of the present invention can include chimeric molecules comprising at least a portion of a FcR that binds to an antibody and a second molecule that enables the chimeric molecule to be bound to a substrate in such a manner that the antibody receptor portion binds to the antibody in at least as effective a manner as a FcR that is not bound to a substrate. An example of a suitable second molecule includes a portion of an immunoglobulin molecule or another ligand that has a suitable binding partner that can be immobilized on a substrate, e.g., biotin and avidin, or a metal-binding protein and a metal (e.g., His), or a sugar-binding protein and a sugar (e.g., maltose).

The present invention includes uses of proteins, antibodies and inhibitory compounds of the present invention for the diagnosis and treatment of allergy and the regulation of other immune responses in an animal.

One embodiment is a therapeutic composition comprising at least one of the following therapeutic compounds: an inhibitory compound of the present invention, a mutein of the present invention, or an antibody of the present invention. Also included is a method to protect an animal from allergy or other abnormal immune responses. Such a method includes the step of administering a therapeutic composition of the present invention to the animal. As used herein, the ability of a therapeutic composition of the present invention to protect an animal from allergy or other abnormal immune responses refers to the ability of that composition to, for example, treat, ameliorate or prevent allergy or other abnormal immune responses. General characteristics of therapeutic compositions and methods to produce and use such therapeutic compositions are disclosed, for example, in WO 98/27208, *ibid.*, see, for example, page 39-47. It is to

be noted that although the compositions and methods disclosed in WO 98/27208, *ibid.*, relate to feline FcεRIα proteins, they are also applicable to therapeutic compositions of the present invention. Therapeutic compositions of the present invention are advantageous because they can be derived from analysis of 3-D models of the present invention and have improved functions, such as efficacy and safety.

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Another embodiment is a diagnostic reagent comprising a mutein of the present invention. As used herein, a diagnostic reagent is a composition that includes a mutein that is used to detect allergy or other abnormal immune responses in an animal. Also included in the present invention are methods, including in vivo methods and in vitro methods, to (a) detect allergy or other abnormal immune response, or susceptibility thereto, in an animal, comprising use of a diagnostic reagent comprising a mutein of the present invention and (b) to enhance the performance of an IgE binding assay, said method comprising incorporating into the assay a mutein of the present invention. General characteristics of diagnostic reagents and methods to produce and use such diagnostic reagents are disclosed, for example, in WO 98/27208, ibid., see, for example, page 2-39. It is to be noted that although the reagents and methods disclosed in 15 WO 98/27208, ibid., relate to feline FcεRIα proteins, they are also applicable to diagnostic reagents, kits and detection methods of the present invention. Muteins of the present invention are advantageous in such applications because of their enhanced affinity for antibodies, altered specificity, enhanced solubility and/or enhanced stability, 20 enabling for example use in otherwise adverse conditions and longer shelf-life.

The following examples are provided for the purposes of illustration and are not intended to limit the scope of the invention.

EXAMPLES

Example 1

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This Example describes the production of a FceRIa nucleic acid molecule, a recombinant molecule, a recombinant cell, a recombinant virus, and a FceRIa protein of the present invention.

A number of human FceRIα proteins of variable lengths (i.e., 171, 172, and 176 amino acids) were produced in a variety of cell lines (i.e., Chinese hamster ovary cells, *Pichia pastoris* yeast, *Spodoptera frugiperda* (Sf9) insect cells and *Trichoplusia ni* (Hi-5) insect cells). Due to a number of factors, however, including protein length, solubility, and extent and variability of glycosylation, only one FceRIα protein was useful in producing a crystal of sufficient quality for the first determination of a model of an extracellular domain of a FceRIα protein. The production of this protein is disclosed below.

A nucleic acid molecule comprising the first 176 amino acids of the mature form of the human FcεRIα protein, nucleic acid molecule and protein designated herein as nhFcεRIα₁₋₅₂₈ and PhFcεRIα₁₋₁₇₆, respectively, was produced as follows. An *Eco*RI-HindIII fragment from plasmid EdpC20 (Blank et al., *ibid.*) containing the human FcεRIα signal sequence and residues 1-172 of the mature human FcεRIα protein was ligated to two oligonucleotides coding for residues 172-176 of the mature protein and two stop codons. The two oligonucleotides, having nucleic acid sequences of 5' AGCTCCGCGT GAGAAGTAAT AAG 3' (SEQ ID NO:5) and 5' GATCCTTATT ACTTCTCACG CuG 3' (SEQ ID NO:6), had *Hin*dIII and *Bam*HI overhangs when annealed together, which permitted the ligation of nhFcεRIα₁₋₅₂₈ into *Eco*RI and *Hin*dIII cleaved baculovirus transfer vector pVL1392 (available from Pharmingen, San Diego, CA) to produce recombinant molecule pVL1392-nhFcεRIα₁₋₅₂₈. The resultant construct was verified by DNA sequencing.

Recombinant virus was produced as follows. Recombinant molecule pVL1392-nhFceRI $\alpha_{1.528}$ was co-transfected with a linear Baculogold baculovirus DNA (available from Pharmingen) into *S. frugiperda* Sf9 cells to form recombinant cell *Sf*9:pVL1392-nhFceRI $\alpha_{1.528}$ which was cultured to produce recombinant virus, namely BV:pVL1392-nhFceRI $\alpha_{1.528}$ using techniques known to those skilled in the art. Supernatants of

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transfected Sf9:pVL1392-nhFceRIa₁₋₅₂₈ cells were amplified once in TNM-FH medium (available from Pharmingen), followed by a second amplification in serum-free medium (SF-900, available from Gibco, Gaithersburg, MD) in a final volume of about 500 milliliters (ml). For Sf9:pVL1392-nhFceRIa₁₋₅₂₈ cells grown in shaker flasks, TNM-FH medium was supplemented with pluronic F-68 (available from Pharmingen). For each virus stock used in protein production, the optimal amount of virus and harvest time post-infection was determined by small scale tests in 50 ml shaker flasks.

Recombinant protein PhFceRIa₁₋₁₇₆ was produced as follows. Trichoplusia ni (Hi-5) cells were infected with recombinant virus BV:pVL1392-nhFcεRIα₁₋₅₂₈ that had been produced as described above to produce recombinant cell Hi-5:pVL1392nhFcεRIα₁₋₅₂₈. Recombinant cell Hi-5:pVL1392-nhFcεRIα₁₋₅₂₈ was grown in shaker or spinner flasks for production of PhFcεRIα₁₋₁₇₆. Typical yields of PhFcεRIα₁₋₁₇₆ were about 2 to 12 milligrams per liter (mg/liter) of infected cells 2 to 4 days after infection.

Recombinant protein PhFceRIa₁₋₁₇₆ was purified as follows. Supernatants from 1.5 to 5 liters of recombinant Hi-5:pVL1392-nhFceRIa₁₋₅₂₈ cells were collected, filtered through 0.2 micron filters, and loaded directly onto a Mab15-1 (Sechi et al., 1996, J. Biol. Chem. 271, 19256-19263) monoclonal antibody column. Supernatants were recirculated over the column at least twice, followed by buffer (100 millimolar (mM) Na, K phosphate, pH 7) washes of about 300 ml, until the absorbance at 280 nanometers (nm) of the eluant returned to zero. PhFceRIa₁₋₁₇₆ was eluted by two urea washes: 100 ml of 5 molar (M) urea in 100 mM phosphate, pH 7.0; then 100 ml of 7 M urea in 100 mM phosphate, pH 7.0; followed by extensive regeneration with 100 mM Na, K phosphate, pH 7.0. The urea eluants were pooled concentrated to about 25 to 40 ml with an Amicon stirring concentrator, and dialyzed 4 times against 2 liters of 50 mM Tris, pH 7.5. The purity of PhFceRI α_{1-176} was verified by SDS-PAGE. Purified PhFceRI α_{1-176} was stored 25 at 4°C in the presence of 0.05% sodium azide. Final yield of PhFceRIa₁₋₁₇₆ was about 50% based on an absorption coefficient of 2.6 mg⁻¹ml for the purified protein and the initial total protein estimated using ELISA assays with the initial cell supernatants.

An inhibition-ELISA assay was used to quantitate PhFceRIa₁₋₁₇₆ expression and yields in initial transfected supernatants, subsequent viral amplifications and large scale protein preparations. In this assay, the binding of Mab15-1 antibody to the plated

PhFceRIα₁₋₁₇₆ protein was monitored using a goat anti-mouse-alkaline phosphatase antibody (A-2429, available from Sigma, St. Louis, MO). Unknown samples were used to compete for antibody binding and compared with a standard curve generated in parallel. Fifty microliters (ml or mL) of purified PhFceRIa₁₋₁₇₆ was incubated in microtiter plates overnight at 4°C at a concentration of 1 mg/ml in phosphate-buffered saline. Plates were rinsed with wash buffer containing 20 mM Hepes, pH 7.5, 100 mM NaCl, 0.1% Tween-20 (Hepes/NaCl buffer) and blocked with Hepes/NaCl buffer containing 1% Carnation dry milk. Standard inhibitor samples ranging from 0.1-50 mg/ml of FhFceRIa₁₋₁₇₆ in two-fold dilution series ware incubated with Mab15-1 (0.1 mg/ml final concentration) and added in duplicate to wells coated with PhFceRIa₁₋₁₇₆. Standard controls included wells without overnight incubation with PhFceRIa₁₋₁₇₆, and addition of Mab15-1 without inhibiting PhFceRIa₁₋₁₇₆. Secondary antibody in a 1:5000 dilution was incubated after washing for 12 hour at room temperature. Plates were washed and developed using the AP reagent p-nitrophenyl phosphate (PNPP, available from Sigma 104-105). Microplates were read using a Molecular Devices SpectraMax Plus reader at 405 nm.

Example 2

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This Example describes the production of a FceRIa protein crystal of the present invention.

Purified PhFceRIa₁₋₁₇₆, produced as described in Example 1, was concentrated to a final concentration of 20 mg/ml in 20 mM Tris pH 7.5. Crystallization was carried out using the hanging drop method, with a precipitant composed of 100 mM Tris, pH 8.5, 200 mM NaOAc, and 18-24% PEG 4000. Crystals were obtained in 2 to 10 days amidst significant amounts of protein precipitate. At lower PEG concentrations, a different crystal form was observed. The crystals used in the structure determination typically grow as clusters of 3 to 20 crystals that could be separated manually. The crystals belong to the monoclinic space group C2, with cell dimensions of 88.6 x 69.6 x 49.3 angstroms, alpha=gamma=90 degrees, beta=116.7 degrees, with one receptor molecule per asymmetric unit. Such crystals diffracted to a resolution of about 2.4 angstroms. Crystals were harvested into harvest buffer containing 35% PEG 4000, 100 mM Tris pH

8.5. It is to be noted that the inventors produced and tested several hundred crystals

using the various other proteins described in Example 1, before successfully obtaining the crystal described immediately above.

Example 3

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This Example describes the production of additional FcεRIα protein crystals of the present invention.

Nucleic acid molecule nhFcεRIα₁₋₅₁₆, encoding the first 172 amino acids of the human FcεRIα protein was expressed in *T. ni* Hi-5 cells to produce PhFcεRIα₁₋₁₇₂ in a manner similar to that described for the production of PhFcεRIα₁₋₁₇₆ in Example 1. Purified PhFcεRIα₁₋₁₇₂ was concentrated to a final concentration of 20 mg/ml in 20 mM Tris pH 7.5. Crystallization was carried out using the hanging drop method, with a precipitant composed of 0.1-0.2 M NaAcetate, 0.1M Na Citrate, pH 5.6, 18-24% PEG, and HECAMEG detergent at it's Critical Micelle concentration (19.5 mM). Crystals were obtained in 2 to 10 days arnidst significant amounts of protein precipitate. The crystals belong to the monoclinic space group P6122 with unit cell dimensions of 58 x 58 x 226 angstroms, alpha=beta=90 degrees; gamma=120 degrees, with one receptor molecule per asymmetric unit. Such crystals diffracted to a resolution of about 3.2 angstroms.

Using a different protocol, purified PhFczRIa₁₋₁₇₆, produced as described in Example 1, was concentrated to a final concentration of 10 mg/ml in 20 mM Tris pH 7.5. Crystallization was carried out using the hanging drop method, with a precipitant composed of 100 mM Tris, pH 7.5, 0-20% isopropanol, and 18-24% PEG 4000. Crystals were obtained in 2 to 10 days amidst significant amounts of protein precipitate. The crystals belong to the monoclinic space group C2, with cell dimensions of 136.02 x 75.01 x 79.28 angstroms, alpha=gamma=90 degrees; beta=117.8 degrees. Such crystals diffracted to a resolution of abent 3.0 angstroms.

Example 4

This Example describes the production of a three-dimensional model of the present invention.

For data collection, crystals, produced as described in Example 2, were mounted in nylon loops (available from Hampton-Research, Laguna Niguel, CA) and rapidly cooled in liquid nitrogen after a short (about 30 second) soak in harvest buffer

supplemented with 14% glycerol. Heavy atom soaks with K₂PtBr₄ and K₃AuCl₃ were done in harvest buffer with 5 mM Pt for 48 hours and 1 mM Au for 18 days. Data were collected at the Stanford Synchrotron Radiation Laboratories (SSRL) 7-1 beamline and at the Dupont-Northwestern-Dow undulator beamline at the Advanced Photon Source at Argonne National Laboratories. The statistics for these data are shown in Table 3.

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Table 3. Crystallographic data and model refinement

	STORES	840 E	PK. C. S.
Resolution	2.4Å	3.0Å	4.0Å
Wavelength/Energy (Å/keV)	1.08/11.48	1.02/12.12	1.05/11.76
Completeness, % (Last Shell)	96.9 (92.5)	99.9 (100.0)	96.3 (69.9)
Ave. Redundancy (Last Shell)	3.9 (3.4)	7.6 (7.3)	6.2 (2.7)
Rmerge, % (last shell)	5.7 (22.6)	10.1 (39.8)	5.1 (7.0)
<i si=""> (last shell)</i>	23.8 (4.5)	19.0 (3.9)	35.2 (15.9)
DF/F (Resolution)		0.218 (20-3Å)	0.093 (20-4Å)
No. of sites	-	1	1
Phasing Power acentric/centric	-	1.50/1.93	0.41/0.61
Rcullis acentric/centric	-	0.66/0.70	0.94/0.97

Overall Figure of Merit

= 0.487

20 FOM after DM =

0.673

Refinement Statistics: 500-2.4Å

Reflections (free) = 10247 (880)
Rfactor/Rfree, % = 24.2/27.1
#atoms = 1620
#waters = 126
RMSD bonds = 0.0077Å
RMSD angles = 1.53°
Ave. B = 65.7Ų

 R_{many} =SII₁-<I>VSIII, where I₁ is the intensity of and individual reflection and <I> is the average intensity of that reflection.

 $R_{wyst} = SIF_p - IF_c / SIF_p$, where F_c is the calculated and F_p is the observed structure factor amplitude. Phasing Power = F_{heat} / E , where $F_{heat} =$ the heavy atom structure factor amplitude and E = the residual lack of closure error.

 $R_{callle} = SliF_{ph} \pm F_{p}l - lF_{beatc}l/SlF_{ph} \pm F_{p}l, \text{ where } F_{ph} \text{ is the derivative structure factor amplitude.}$

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For the Pt and Au datasets, the wavelength was chosen to be 200 eV above the absorption edge of the metal, in order to maximize the anomalous signal for each heavy atom. Heavy atom data were collected using reverse beam protocols to optimize the anomalous diffraction signal. Diffraction data were collected with a Mar300 Image plate (SSRL) or a MarCCD detector (DND-CAT), and integrated and scaled with DENZO/SCALEPACK; see, Otwinowski et al., 1997, In Methods in Enzymology:

Macromolecular Crystallography, part A, Academic Press, pp 307-326. The CCP4 suite of programs (Collaborative Computational Project, 1994, Acta Cryst. D50, 760-763) was used for further processing and identification of heavy atom sites.

10 Heavy atom positions were identified from peaks in the anomalous and isomorphous difference patterson maps. Heavy atom positions were refined and phases calculated with the program MLPHARE, followed by solvent flattening and density modification with the program DM (Collaborative Computational Project, 1994, ibid.). The subsequent model was using the CNS program (Brunger et al., 1998, Acta Crystallogr D Biol Crystallogr 54, 905-921) with the combined maximum likelihood and experimental phase target (MLHL). Specifically, the structure of the FceRIa protein PhFceRIa₁₋₁₇₆ was determined by multiple isomorphous replacement using gold and platinum heavy atom derivatives with the anomalous signal from both derivatives. The data collection and heavy atom phasing statistics are shown in Table 3. The MIRAS phases were used as input to the density modification program DM and the electron 20 density map was of sufficient quality that the entire model except for two flexible loops and five residues at the termini could be built; see Fig. 1A and 1B. The model was further improved by cycles of automated refinement using the program CNS followed by manual rebuilding. The current R-factor and Rfree are 24.2% and 27.1% respectively for all the data to 2.4 angstroms. No electron density was observed for three residues at the N-terminus (1-3) and 2 residues at the C-terminus (175-176), and poor density was observed for two loops (residues 32-35 and 70-73) that are disordered in the crystal. Final statistics for the model are shown in Table 3.

Example 5

This Example describes the structure of a FcεRIα protein predicted by a threedimensional model of the present invention.

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A. Overall structure

The model of extracellular domain of the human FceRIa protein, also referred to herein as the hFceRIa model or hFceRIa structure, indicates that PhFceRIa is composed of two immunoglobulin (Ig) domains, D1 and D2, each about 85 residues in length, that are bent at an acute angle relative to each other and form an extended convex surface; see Fig. 2. The domain arrangement generates a flat surface at the top of the receptor that has been implicated in binding to the Fc domain of an igE antibody. The domains are small compared to canonical variable and constant Ig domains and the shorter sequence is accommodated by truncation of the CC'E crossover region; see Fig. 2. Both domains D1 and D2 of the hFceRIa model are composed of beta-strands AA'BCC'EFG, differing from the previously described I-set domains (Harpaz et al., 1994, J. Mol. Biol. 238, 528-539) by the absence of strand D. The nearly antiparallel domain packing places the A'B, CC' and EF loops of D1 and the BC, C'E and FG loops of D2 near the top of the receptor; see Fig. 2. One feature of the topology is a crossover 15 of the A strand from the ABE sheet to the CC'FG sheet, forming a short segment of parallel beta sheet in an otherwise antiparallel structure; see Fig. 2 and Fig. 3. In D1, the AA' crossover make contacts in the D1D2 interface (see below), while in the D2

Significant structural differences are also observed between D1 and D2 of the hFceRIα model. The D1 and D2 sequences contain about 28% identical residues and superimpose with an RMS deviation of 1.2 angstroms for the Ca atoms. The F-G strands and loop differ between the two domains. In D2, these strands are longer and the FG loop projects above the D2 domain surface. The C' strands also differ between the two domains. In D2, a series of aromatic residues (tyrosines at positions 120 and 131) form a hydrophobic core that pushes the C' strand and loop away from the C strand, altering the local conformation of this region. The FG loop and C-C' strands of D2 form part of the binding site for IgE (see below).

domain, residues in the A strand interact with D1; see Fig. 3.

The tertiary packing arrangement of the hFceRI\alpha D1 and D2 domains is distinct from other tandem Ig domain structures; see Fig. 4. Comparison of the hFceRI\alpha model with other bent two-Ig domain structures reveals a high degree of variability in the bend angles and packing surfaces between domains. A subset of D1 and D2 representative

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structures of are shown in Fig. 4, including those from human FceRIa (designated as IgE-FcR), the natural killer cell inhibitory receptor, (KIR, Fan et al., 1997, Nature 389. 96-100), the human growth hormone receptor (HGHBP, de Vos et al., 1992, Science 255, 306-312), the interleukin-1 receptor, (IL1R, Vigers et al., 1997, Nature 386, 190-194) and the insect defense protein hemolin (Su et al., 1998, Science 281, 991-995). The structures are oriented similarly with respect to the carboxyl-termini of the two Ig domains being compared. The figures on top show side views and the figures below show top views. The FceRIa and hemolin structures have the most acute angles relating two sequential Ig domains. The top view of these domains shows that the orientation of the hemolin and FceRIa domains are more closely related, but between this selected subset of proteins there is significant variability in the relative orientations of tandem Ig domain structures. The bend angle between domains and domain packing interfaces are clearly unique, and this variation is likely to be important in ligand binding interactions. For example, the FG loop of D2 in hFceRIa is oriented quite differently with respect to D1 residues as compared to the same region of the KIR or HGHBP, thus changing the spatial relationships of D1D2 loops that may be involved in ligand interactions. To the inventors' knowledge, the hFceRIa structure defines a new group of two sequential Ig domain structures that differs from other known tertiary arrangements.

B. The D1D2 interface

The bent shape of the FceRIα structure produces a large interface between the D1D2 domains that buries 1280 Ų of accessible surface area of 28 D1D2 residues. There are 11 residues from the D1 domain (12-18, 20, 84-86) and 17 residues from the D2 domain that are buried at the interface (87-93, 95, 104, 106, 108, 110-111, 161, 163-165). Of these 28 residues, 8 are completely conserved in all human FcgR and FceRIα sequences (corresponding to residues 13, 87, 88, 90, 91, 106, 108, 110 of SEQ ID NO:2); see Fig. 5. These conserved residues form a significant fraction to one side of the buried interface, suggesting that related FcRs would have a similar acute packing of the D1D2 domains as observed in the FceRIα model.

However, 20 residues that form the D1D2 interface in the FcεRIα model differ in other FcRs and these differences could alter the relative orientations of the two domains. For example, the conserved tryptophan at position 110 packs against a phenylalanine at

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position 17 of FcεRIα. In related FcRs, this phenylalanine is changed to a leucine, which may lead to slight alterations in the packing of the two domains. Another central residue in the FcεRIα D1D2 interaction is residue R15, which forms a hydrogen bond with the carbonyl of L90 and is packed against L89, F84, and L165. In related human FcRs, arginine 15 is changed to serine or asparagine, which corresponds to a significant volume and charge change at the center of the D1D2 interaction. Since the interactions of the FcR with antibody are near the D1D2 interface, alterations in residues at the interface might influence receptor specificity. Other residues that are variable amongst the FcR sequences in the region of the D1D2 could also perturb the D1D2 interactions.

The bent hFceRIα structure generates a cleft between the two domains that is near the trans-membrane anchor at the C-terminus of D2; see Fig. 2. This cleft is located far from the IgE binding site identified by mutagenesis studies (see below). Although there is no known function attributed to this region, while not being bound by theory, it is believed that this region could be a site of interaction with the extracellular regions of the beta or gamma subunits of the receptor. It has been suggested that interactions between the FcgRI and FcgRIIIA alpha and gamma subunits increase the binding affinity of the receptor for IgG (Miller et al., 1996, *J. Exp. Med. 183*, 2227-2233). Although the extracellular regions of the human FceR gamma chain are short (about 5 to 7 amino acids), these regions could potentially interact with the D1D2 cleft and thereby affect the affinity of the receptor for antibody. In addition, recent binding studies with recombinant, soluble FceRIα and IgE have demonstrated a 10-fold lower affinity than had previously been determined in cell-binding assays (Cook et al., 1997, *ibid.*).

C. Carbohydrate attachment sites

The human FceRIα protein PhFceRIα₁₋₁₇₆ is the most highly glycosylated protein structure solved by X-ray crystallography to date, having seven N-linked glycosylation sites in 176 amino-acid residues. The intact FceRIα on mast cells is approximately 40% carbohydrate by weight (Kanellopoulos, et al., 1980, E. J. Biol. Chem. 255, 9060-9066); LaCroix, et al., 1993, *ibid.*), with a heterogeneous molecular weight on SDS-PAGE gels of about 50 kilodaltons (kD). Human FceRIα expressed in insect cells has a molecular weight of about 34 kD as observed using SDS-PAGE, but, based on typical insect cell glycosylation structures (-GlcNAc₂-Man₃-GlcNAc), could be expected to have a

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molecular weight of about 27.5 kD, suggesting the protein is about 30% carbohydrate by weight. While the presence of carbohydrate at the seven N-glycosylation sites is not required for binding to IgE (Letourneur et al., 1995, *ibid.*; Robertson, 1993, *ibid.*; Scarselli et al., 1993, *ibid.*), mutation of these sites or treatment of FceRI-expressing cells with tunicamycin leads to the aggregation of the receptor during biosynthesis.

In the hFcεRIα structure, carbohydrate density is observed at three of the seven predicted glycosylation sites. For two of these sites, asparagines 42 and 166, three sugar moieties were built. The carbohydrate at position 42 extends up towards the top of the FcεRIα structure, covering residues F60, S63 and V83. The carbohydrate attached to position 166 projects away from the protein surface, potentially as a result of crystal contacts and the modification of the third and sixth positions of the first GlcNac residue. The third carbohydrate attachment site is the arginine at position 21.

Many of the related FcR proteins are also highly glycosylated proteins and the glycosylation sites vary between receptors. Rat and mouse FcεRIα proteins each have six potential N-linked glycosylation sites, of which two sites and one site, respectively are shared in common with the human FcεRIα protein. Comparison of seventeen human and animal FcR sequences identifies twenty-five different potential N-linked carbohydrate attachment sites in related FcRs. The twenty-five sites are distributed evenly between D1 and D2, with fourteen sites in D1 and eleven sites in D2. Five of these sites are relatively well conserved sites in all FcRs (found in > 9/17 sequences analyzed) and they correspond to residues 35, 42, 61, 135, and 142 of SEQ ID NO:2. These sites cover a significant fraction of the FcεRIα surface on both major faces of D1 and D2, placing limitations on the surface available for interactions with antibody.

It is not known why FcRs are so heavily glycosylated. Many potential roles for carbohydrate sites on proteins have been suggested, including specific roles in determining the tertiary (Wyss et al., 1995, Science 269, 1273-1278) or quaternary structures of proteins (Huber et al., 1976, Nature 264, 415-420; Vaughn et al., 1998, Structure 6, 63-73). In the case of the human FcRs, the number of potential N-linked glycosylation sites correlates to some degree with the affinity of the FcR for immunoglobulin. Table 4 shows the number of glycosylation sites in the domains corresponding to the extracellular domain of the human FceRIa protein along with the

total number of glycosylation sites in parentheses. Affinity data are taken from Ravetch et al., 1998, *ibid.*; Ravetch et al., 1991, *Annu. Rev. Immunol.* 9, 457-492.

Table 4. Comparison of the number of predicted glycosylation sites and the affinity of different FcRs for antibody.

TAR ME	(G)(0)((E)	Winity.
	<u>Human</u>	
FceRI	7	high (10 ⁻⁹ -10 ⁻¹⁰ M)
FcγRIA (CD64)	5 (7)	high (3 domains, 10 ⁻⁸ -10 ⁻⁹ M
FcyRIB (CD64)	5 (7)	high (3 domains, 1)-8-10-9M
FcyRIIA (CD32)	2 (3)	low (10 ⁻⁶ M)
FcyRIIB (CD32)	3	low (10 ⁻⁶ M)
FcyRIIC (CD32)	3 (4)	low (10 ⁻⁶ M)
FcyRIIIA (CD16)	5 (6 in variant)	low (10⁴M)
	Mouse	
FceRI	6	high (10 ⁻⁹ -10 ⁻¹⁰ M)
FcγRI	4(5)	high (3 domains, 10 ⁻⁷ -10 ⁻⁸ M)
FcγRIIb	4(5)	low (10-6M)
FcγRIIIa	4	low (10 ⁻⁶ M)
	Rat	
FceRI	7	high (10 ⁻⁹ -10 ⁻¹⁰ M)
FcγRII	6 (7 total)	low
FcγRIII	5	low
	Other	
FcyRII (guinea pig)	5(6)	low
FcγRIII (pig)	3	low
FcyRII (bovine)	6	low

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In the high affinity FcRs, there are typically 5 to 7 potential N-linked glycosylation sites, whereas in the low affinity FcRs there are as few as two sites. One significant difference in the function of the high and low affinity FcRs is the probability that they will bind antibody in the absence of antigen. The high affinity receptors such as FceRI can bind IgE prior to interacting with antigens. While not being bound by theory, it is believed that since FcR activation requires crosslinking of receptors, glycosylation might prevent the aggregation of large antibodies at the cell surface bound by FcRs. Crystallization of proteins at lipid/water interfaces can occur readily, and the potentially high local concentrations of membrane-bound antibodies might lead to FcR activation in the absence of antigen. The low affinity IgG receptors interact with antibody-antigen aggregates that can simultaneously bind and activate multiple FcRs. While not being bound by theory, it is believed that glycosylation may not be quite as important for these receptors, since interaction with the antibody could occur after the binding of antigen.

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However, it is likely that there are additional explanations for the glycosylation that is observed in the FcRs. The non-human FcRs do not show an obvious correlation of the number of carbohydrate sites and FcR affinity. While not being bound by theory, it is believed that glycosylation might be important in FcR signaling, by orienting receptor:antibody complexes into functional signaling complexes (i.e. by preventing antigen-crosslinked complexes from forming non-functional aggregates). It is known that activation through FceRI is sensitive to some geometrical constraints imposed by antigen crosslinkers, although the nature of these physical constraints is poorly understood. The recent crystal structure determination of an erythropoietin-receptor complex suggests that the orientation of ligand-mediated dimerization of cell-surface receptors may be important in efficient signal transduction (Syed et al., 1998, *Nature* 395, 511-516).

D. Receptor binding site for IgE (IgE binding domain)

A number of mutagenesis studies have been carried out in an effort to elucidate the regions of the FceRI that are critical for the interaction with IgE molecules (Cook et al., 1997, *ibid.*; Hulett et al., 1993, *ibid.*; Hulett et al., 1994, *ibid.*; Hulett et al., 1995; Mallamaci et al., 1993, *ibid.*). These experiments have demonstrated an important

role for amino acids in the D2 domain of the receptor, although some regions of D1 are also likely to be involved in IgE binding. Studies suggesting that D1 plays a role in IgE binding include the deletion of D1 (Robertson, 1993, *ibid.*; Scarselli et al., 1993, *ibid.*) or substitution with a homologous IgG receptor (Hulett et al., 1994, *ibid.*). These experiments do not determine conclusively whether D1 interacts directly with the IgE or whether D1 indirectly alters the structure of D2 and subsequent interactions with IgE. Analysis of the hFceRIa model of the present invention is needed to predict important IgE binding regions in the protein. For example, the substitution or elimination of residues at the D1D2 interface can influence D2 interactions with antibody Fc regions.

In addition, there are a number of regions of D1 which have been excluded as determinants of the specificity of the receptor for IgE, since these FcεRIα segments can be substituted by the corresponding residues in the FcgRIIIA protein (Mallamaci et al., 1993, *ibid.*). These residues include segments 25-38, 43-54, 67-79, and 77-86. Substitution of residues 10-21 or 55-67 disrupt the binding of IgE and 5 different monoclonal antibodies, suggesting that residue differences in these segments may affect the folding of hybrid molecules. The 3-D models of the present invention, however, are needed to conduct an amino acid by amino acid analysis of which residues actually directly interact with IgE antibodies.

The FceRIα residues which have been implicated in past studies include residues in the D2 BC loop (amino acid 115), in the C strand (amino acids 117, 118, 120-123), in the C'E loop (amino acids 129, 131), the F strand (amino acids 149, 153) and the FG loop (amino acids 155 and 159) (Cook et al., 1997, *ibid.*; Hulett et al., 1994, *ibid.*; Hulett et al., 1995, *ibid.*). In addition, residues 87 (at the D1D2 interface) and 128 (in the C'E loop) are likely to be part of the IgE interaction site, since mutation of these residues have been shown to influence receptor binding to the IgE point mutant R334A (Cook et al., 1997, *ibid.*). Furthermore, a synthetic peptide corresponding to residues 119-129 has been demonstrated to block IgE binding to the FceRIα, with an apparent K_D of about 3 mM (McDonnell et al., 1997, *ibid.*; McDonnell et al., 1996, *ibid.*).

Analysis of the hFcεRIα model, however, is needed to indicate that of the fifteen residues (i.e., amino acids 87, 115 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159), six are buried in the protein core (i.e., amino acids 115, 118, 120, 131, 149, 155)

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and predicts that substitution at these positions may lead to indirect structural changes that affect IgE binding. Three of the residues are either partially buried or glycine (i.e., amino acids 122, 129, 153), and substitution may affect the conformation of the local residues. The remaining residues (i.e., amino acids 87, 117, 121, 123, 128, 159) are all exposed amino acids at the FceRIa surface. All of the implicated residues form a contiguous surface extending from the back side of the D2 domain to the top region near the D1D2 interface. Four of the residues are conserved in all human FcRs (i.e., amino acids 87, 118, 149, and 153) and may define a set of common interactions between all FcR receptors and their target Ig molecules.

The hFcεRIα model also indicates that the region of the D2 domain defined by mutagenesis also borders on a number of surface accessible aromatic residues, including four prominent tryptophans at the top of the FcεRIα molecule, namely residues 87, 110, 113, and 156. These four tryptophans form a flat, hydrophobic ridge that neighbors the D2 FG loop. This unusual arrangement of four surface tryptophans probably forms a contact surface for a complementary interaction with an IgE antibody. Tryptophan 87 has already been implicated by mutagenesis studies and tryptophan 156 is prominently displayed at the top of the FG loop. Tryptophan 156 is a glycine in all FcgRs and grafting of residues 154-161 of the FcεRIα FG-loop to FcgRII confers IgE binding. It is to be noted, however, that such a graft does not eliminate IgG binding. The hFcεRIα model predicts that other amino acids, e.g., the tryptophan at residue 87, may be important for antibody class recognition specificity. Other exposed aromatic residues are found concentrated near the IgE binding domain; Fig 6 shows a surface representation of all of the exposed aromatic groups in the hFcεRIα structure, clearly outlining the tryptophan ridge and residues in D2 near the CC'E region.

25 E. Implications for the binding of other FcRs

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Since carbohydrate would be expected to disrupt any close-packed protein:protein interface, it is interesting to compare the known carbohydrate sites with the proposed IgE-binding site on the receptor surface as defined by models of the present invention. The positions of the carbohydrate attachment sites for seventeen related FcRs indicated that the N-linked carbohydrate sites delineate a boundary around the proposed IgE binding site. This is consistent with the suggestion that related FcRs share a

common binding surface for antibody molecules. Studies of the FcgRII specificity for IgG, for example, have implicated the following residues: amino acids 113-116, 129, 131, 133, 134, 155, 156, and 159-161 (Hulett et al., 1994, *ibid.*; Hulett et al., 1995, *ibid.*). In addition, domain-swap experiments have demonstrated that two of the related FcgRs can form functional hybrid molecules with FcεRIα (Hulett et al., 1995, *ibid.*; Mallamaci et al., 1993, *ibid.*), suggesting that these receptors share a common binding surface with their respective antibody ligands. Once again, however, it should be noted that only with the model can one predict exactly which FcR residues directly interact with an Fc domain of an antibody.

The hFceRIa model indicates that the top of the FcR structure is devoid of carbohydrate-attachment sites in the region of D2 that has been implicated in direct interactions with Ig molecules. The neighboring surface of the D1 domain including loops A'B and EF, are also devoid of carbohydrate and could form part of an extended antibody binding site across the D1D2 interface. If these D1 loops are important in determining the specificity and affinity of the FcR:antibody interaction, one might observe sequence variability between high affinity and low IgG receptors and the IgE receptor. This variability in the human IgG and IgE receptors is shown in Fig. 5. For residues 3-173 of the hFceRIa protein, there are 73 amino acid differences that are unique to the IgE receptor as compared to any of the IgG receptors and these are indicated below the sequence alignments. Of these 73 amino acids unique to the human FceRIa protein, 27 positions are highly variable in the different FcR sequences (> 4/7 different amino acids. There are five regions that stand out with clusters of variable residues: residues 27-30, 47-49, 54-33, 94-98 and 155-159. Residues 155-159 (the FG loop) are highly variable and do at least partially determine the specificity of FcR interactions. It is again to be noted that without the model one cannot determine which regions of sequence variability are important in determining FcR protein functional domains.

Previous experiments have shown that residues 27-30 and 47-49 are not critical for FcR specificity (Mallamaci et al., 1993, *ibid.*), and the presence of glycosylation sites within these segments in related FcRs support the suggestion that these regions are not part of the FcR:antibody interaction. The hFccRIα model indicates that residues 94-98

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are found in the A' strand near the D1D2 cleft and therefore are not likely to interact with antibody directly, but these residues might influence interactions indirectly by altering the D1D2 packing interface.

The remaining group of highly variable residues (54-59) are in the D1 E strand (see Fig. 7), near the FcεRIα binding site as predicted by the hFcεRIα model. Residues 54-59 could form a D1 surface of interaction with the Fc domains of antibodies, extending the binding site across both FceRIa domains. This prediction is supported by a study reporting that the exchange of FceRIa residues 55-67 with residues from the FcgRIIIA receptor disrupts the folding of the protein (Mallamaci et al., 1993, ibid.), as some of the residue changes form part of the D1 hydrophobic core. The hFceRIa model also predicts that the neighboring D1 A'B loop (residues 18-21) could also form part of an extended surface of interaction with the antibody. Thus, models of the present invention are needed to interpret data from mutagenesis and swapping experiments.

F. Stoichiometry of binding between FcR and antibody

The activation of FcR-bearing cells requires crosslinking of the receptors, which leads to the activation of intracellular kinase cascades analogous to those in B and T cells. For both high and low high affinity receptors FceRI and FcgRIII, a stoichiometry of 1:1 is observed between the receptor and the Fc domains of the respective antibodies to which they bind (Ghirlando et al., 1995, Biochemistry 34, 13320-13327; 20 Kanellopoulos et al., 1980, ibid.; Keown et al., 1997, Eur. Biophys. J. 25, 471-476), consistent with a requirement for antigen to cause receptor aggregation and activation. The binding site on the Fc domain of an IgE antibody for its receptor has been extensively studied by mutagenesis, implicating amino acids in the third constant domain (Ce3) of the IgE (Basu et al., 1993, J. Biol. Chem. 268, 13118-13127; Henry et al., 1997, Biochemistry 36, 15568-15578; Nissim et al., 1991, Embo J. 10, 101-107; Presta et al., 1994, J. Biol. Chem. 269, 26368-26373). The structure of the Fc domain of IgE antibodies (also referred to as IgE-Fc domains) has not been experimentally determined, but is homologous to the Fc domain of IgG antibodies (also referred to as IgG-Fc domains), for which a number of crystal structures are available (Harris et al., 30 1998, J. Mol. Biol. 275, 861-872; Huber et al., 1976, Nature 264, 415-420). The residues of the IgE-Fc domain implicated in binding to FceRs based on mutagenesis

analysis are shown mapped onto the structure of the IgG-Fc domain in Fig. 8. The site on an IgG-Fc domain to which FcgRI and FcgRII receptors bind has been mapped to a similar, although smaller, surface that primarily includes residues in the hinge region before the Cg2 domain (Canfield et al., 1991, *J. Exp.Med. 173*, 1483-1491; Duncan et 5 ...a.., 1988, *Nature 332*, 563-564; Jefferis et al., 1990, *Mol. Immunol. 27*, 1237-1240; Lund et al., 1991, *J. Immunol. 147*, 2657-2662).

An antibody Fc domain is a homodimeric structure that is significantly larger than its respective FcR; see Fig. 8. The observed 1:1 stoichiometry between receptor and antibody indicates that the two-fold symmetry of the Fc domain does not lead to the binding of two FcRs, even with isolated molecules in solution. Without being bound by theory, it is believed that the large and convex nature of the FcR binding surface could span two antibody domains (Cg2 in IgG and Ce3 in IgE) and induce a conformational change in the Fc domain that would prevent the binding of a second FcR to the same antibody. The FcR structure could also form an asymmetric complex with the antibody that sterically blocks the binding of a second FcR, perhaps using the protruding FG loop to block symmetric interactions with the Fc hinge region.

Example 6

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This Example describes the production of additional three-dimensional models of the present invention as well as descriptions of FceRIa proteins predicted therefrom.

A. Production and description of a crystal of PhFc ϵ RI α_{1-172} that belongs to tetragonal space group P4₃, with a=b=145.08Å, c=62.74Å, a=b=g=90°, referred to herein as crystal form T1

Protein PhFceRIa₁₋₁₇₂, having SEQ ID NO:4, was produced using techniques known to those skilled in the art by a lec1 Chinese hamster ovary (CHO) cell line transformed with a nucleic acid molecule encoding the protein, i.e., a nucleic acid molecule comprising SEQ ID NO:3. Crystals were grown in a manner similar to that described in Example 2 via vapor diffusion using a well solution of 20% to 32% PEG 10000, 0.1 M ammonium citrate pH 5.6, and 0.1 M sodium chloride, and a protein starting concentration of 5 to 10 mg/ml. Other size PEGs from 4000 to 20000 were also used, as well as sodium citrate pH 5.6 as a buffer. Other salts such as sodium acetate and ammonium sulfate were also used to grow crystals. The crystal used in the structure

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determination, analyzed in a manner similar to that described in Example 4, had five copies of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.1Å. This crystal form, form T1, was refined to a crystallographic $R_{\text{free}}/R_{\text{work}}$ of 32.78%/29.19% using all the observed data |F| > 0 to 3.1Å and a non-crystallographic symmetry (NCS) restraint constant of 300 kcal/mol Å² for all atoms. There were no waters included in the model. The atomic coordinates of PhFceRIa₁₋₁₇₂, form T1, are listed in Table 5. The solvent accessibilities of the amino acids of PhFceRIa₁₋₁₇₂, form T1, are indicated in Table 9. Table 13 provides crystallographic data and model refinement statistics of PhFceRIa₁₋₁₇₂, form T1. A root mean square (rms) deviation analysis of the alpha carbon positions of PhFcεRIα₁₋₁₇₂, form T1, as compared to PhFceRIa₁₋₁₇₆, form M1, is shown in Table 14. The first line is an overall rms on the segments that align in space. The second two lines are the rms deviations for the loops when the molecules are superimposed according to the first line. Only one copy of model in T1 is compared because the models do not differ by much because of tight NCS restraints.

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B. Production and description of a crystal of PhFceRI α_{1-172} that belongs to tetragonal space group P4₃, with a=b=150.50Å, c=74.18Å, $\alpha=\beta=\gamma=90^{\circ}$, referred to herein as crystal form T2.

Protein PhFceRIa₁₋₁₇₂, having SEQ ID NO:4, was produced using techniques known to those skilled in the art by a lec1 Chinese hamster ovary (CHO) cell line transformed with a nucleic acid molecule encoding the protein, i.e., a nucleic acid molecule comprising SEQ ID NO:3. Crystals were grown and analyzed as described in Example 6A. The crystal used in the structure determination had five copies of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.8Å. This crystal form, form T2, was refined to a crystallographic R_{free}/R_{work} of 30.64%/27.99% using all the observed data |F| > 0 to 3.8Å and a NCS restraint constant of 300 kcal/mol $Å^2$ for all atoms. There were no waters included in the model. The atomic coordinates of PhFceRIa₁₋₁₇₂, form T2, are listed in Table 6. The solvent accessibilities of the amino acids of PhFceRI α_{1-172} , form T2, are indicated in Table 10.

Table 13 provides crystallographic data and model refinement statistics of PhFceRIa₁₋₁₇₂, 30

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form T2. A rms deviation analysis of the alpha carbon positions of PhFceRI α_{1-172} , form T2, as compared to PhFceRI α_{1-176} , form M1, is shown in Table 14.

C. Production and description of a crystal of PhFc ϵ RI α_{1-176} that belongs to monoclinic space group C2, with a=136.90Å, b=73.79Å, c=79.40Å, $\alpha=\gamma=90^{\circ}$, and $\beta=117.74^{\circ}$, referred to herein as crystal form M2.

Protein PhFceRIa₁₋₁₇₆, having SEQ ID NO:2, was produced in T. ni Hi-5 cells as described in Example 1. Crystals were grown in a manner similar to that described in Example 2 via vapor diffusion using a well solution of 12% to 20% PEG 4000, 0.1 M HEPES (or Tris) pH 7.5, and 0 to 10% isopropanol, and a protein starting concentration of 5 to 30 mg/ml. The crystal used in the structure determination, analyzed in a manner similar to that described in Example 4, had two copies of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.2Å. This crystal form, form M2, was refined to a crystallographic $R_{\text{free}}/R_{\text{work}}$ of 28.30%/25.69% using all the observed data |F| > 0 to 3.2Å. A NCS restraint constant of 300 kcal/mol Å² has been imposed for all atoms except certain ones in loops and crystal contacts (residues 1-3, 27-38, 41-43, 69-75, 87, 98, 111-117, 125-135, 144, 152-158 of SEQ ID NO:2) and the N-linked carbohydrate atoms. There were no waters included in the model. The atomic coordinates of PhFceRIa₁₋₁₇₆, form M2, are listed in Table 7. The solvent accessibilities of the amino acids of PhFceRIa₁₋₁₇₆, form M2, are indicated in Table 11. Table 13 provides crystallographic data and model refinement statistics of PhFceRIa₁₋₁₇₆ form M2. A rms deviation analysis of the alpha carbon positions of PhFceRIα₁₋₁₇₆, form M2, as compared to PhFceRIα₁₋₁₇₆, form M1, is shown in Table 14.

D. Production and description of a crystal of PhFceRI α_{1-172} that belongs to hexagonal space group P6₁22, with a=b=58.62Å, c=229.19Å, α = β = γ =90°, referred to herein as crystal form H1.

Protein PhFcεRIα₁₋₁₇₂, having SEQ ID NO:4 except that the isoleucine at position 170 was replaced with cysteine, was produced in a manner similar to that described in Example 1, except that Spodoptera frugiperda Sf9 cells were used instead of T. ni Hi-5 cells. Crystals were grown in a manner similar to that described in Example 2 via vapor diffusion using a well solution of 20% to 30% PEG 4000, 0.1 M sodium citrate pH 5.6,

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- 0.1 M sodium chloride, and 5-40mM Methyl-6-O-(N-heptylcarbamoyl)-a-D-glucopyranoside (HECAMEG), a protein starting concentration of 10 mg/ml. The crystal used in the structure determination, analyzed in a manner similar to that described in Example 4, had one copy of the receptor in the crystallographic asymmetric unit and diffracted to a maximum resolution of 3.2Å. This crystal form, form H1, was refined to a crystallographic R_{free}/R_{work} of 31.27%/28.78% using all the observed data |F| > 0 to 3.2Å. The atomic coordinates of PhFceRI α_{1-172} , form H1, are listed in Table 8. The solvent accessibilities of the amino acids of PhFceRI α_{1-172} , form H1, are indicated in Table 12. Table 13 provides crystallographic data and model refinement statistics of PhFceRI α_{1-172} , form H1. A rms deviation analysis of the alpha carbon positions of PhFceRI α_{1-172} , form H1, as compared to PhFceRI α_{1-176} , form M1, is shown in Table 14.
- E. The principal differences in the structures from the various crystal forms occurred in the BC loop in domain 1 (the "30 loop"), the C' strand in domain 2 (the "130 region") and the carbohydrate sites. There were also smaller differences in the termini of the structures and the FG loop in domain 1 (the "72 loop").

The 30 loop showed the greatest variability across the different space groups. The density for this loop was often the poorest density in the map, suggesting that the loop may vary in conformation even within a single crystal. In T1 and T2, the density for this loop was higher than the rest (when the molecule was viewed in the normal orientation, with the FG loop of domain 2 at the top and the cleft between the domains at the bottom.) In the tetragonal cells, the 30 loop passed close to residue 51. In the two copies of the receptor in the larger monoclinic cell M2, the 30 loop was pulled down by crystallographic contacts. In these two copies, the density for the 30 loop clearly showed the loop was pulled away from the rest of the molecule to reveal an empty space inside the loop. The location of the 30 loops in H1 and M1 was intermediate to those of the tetragonal cells and M2.

The 130 strand varied across the crystal forms as well. In T1, T2, and the B copy in M2, this strand hydrogen bonded with the C strand in domain 2 to form a canonical C' strand. In the H1 form, the strand crossed over to the other side of the sheet to form a D strand. In the forms M1 and the A copy of M2, this strand was intermediate to a canonical C' and D strand.

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The density at the termini tended to be poorly ordered, but the M2 crystal showed density for the N-terminus. All of the other models began at amino acid 4. The M1 and M2 models were built to residue 174 out of 176 total residues, the H1 model was built to the C-terminal residue 172, and the two tetragonal forms have models that were built to residue 171 out of 172 total residues.

Table 5. Atomic coordinates of PhFceRI α_{1-172} , Form T1

	ATOM	MOTA							
	NUMBER	TYPE	RESIDUE	#	<u> </u>	<u> </u>		<u>000</u>	<u>B</u>
5	1 2	CB CG	LYS C	4	14.321	45.864	45.068	1.00	151.11
,	3	CD	LYS C LYS C	4	15.396	44.904	44.650	1.00	151.11
	4	CE	LYS C	4	16.203 17.285	44.418 43.425	45.852 45.453	1.00 1.00	151.11
	5	NZ	LYS C	4	18.066	42.968	46.639	1.00	151.11 151.11
10	6	C	LYS C	4	12.828	45.080	43.246	1.00	214.46
10	7 8	0	LYS C	4	12.702	44.022	43.863	1.00	214.46
	9	N CA	LYS C LYS C	4	12.367	47.226	44.431	1.00	214.46
	10	N	PRO C	5	13.426 12.448	46.310 45.209	43.920 41.965	1.00	214.46
	11	CD	PRO C	5	12.271	46.470	41.224	1.00 1.00	98.70 125.98
15	12	CA	PRO C	5	11.863	44.086	41.229	1.00	98.70
	13 14	CB	PRO C	5	10.998	44.785	40.181	1.00	125.98
	15	CG C	PRO C PRO C	5 5	11.793	45.997	39.866	1.00	125.38
	16	ŏ	PRO C	5	12.912 14.063	43.157 43.545	40.611 40.398	1.00	98.70
20	17	N	LYS C	6	12.509	41.923	40.330	1.00 1.00	98.70 208.77
	18	CA	LYS C	6	13.417	40.948	39.747	1.00	208.77
	19	CB	LYS C	6	14.011	40.068	40.851	1.00	249.20
	20 · · 21	CG	LYS C	6	15.074	39.104	40.363	1.00	249.20
25	22	CD CE	LYS C LYS C	6 6	15.769	38.385	41.512	1.00	249.20
	23	NZ	LYS C	6	16.860 17.633	37.456 36.780	40.986 42.068	1.00	249.20
	24	C	LYS C	6	12.709	40.087	38.703	1.00 1.00	249.20 208.77
	25	0	LYS C	6	11.779	39.341	39.022	1.00	208.77
30	26	N	VAL C	7	13.159	40.207	37.454	1.00	73.65
30	27 28	CA CB	VAL C	7	12.599	39.454	36.315	1.00	73.65
	29	CG1	VAL C VAL C	7 7	13.163 12.395	39.923 39.255	34.968	1.00	90.39
	30	CG2	VAL C	7	13.095	41.425	33.860 34.847	1.00 1.00	90.39 90.39
25	31	С	VAL C	7	12.876	37.955	36.338	1.00	73.65
35	32	0	VAL C	7	14.017	37.539	36.224	1.00	73.65
	33 34	N	SER C	8	11.833	37.148	36.461	1.00	91.19
	3 4 35	CA CB	SER C SER C	8	12.002	35.707	36.469	1.00	91.19
	36	OG	SER C	8 8	11.113 9.751	35.074 35.407	37.541	1.00	89.05
40	37	c	SER C	8	11.625	35.174	37.345 35.091	1.00 1.00	89.05 91.19
	38	0	SER C	8	10.978	35.870	34.308	1.00	91.19
	39	N	LEU C	9	12.047	33.946	34.794	1.00	76.39
	40 41	CA	LEU C	9	11.750	33.300	33.511	1.00	76.39
45	42	CB CG	LEU C	9 9	13.016	33.111	32.687	1.00	48.15
	43	CD1	LEU C	9	13.863 14.684	34.301 33.924	32.245 31.048	1.00	48.15
	44	CD2	LEU C	9	12.964	35.448	31.863	1.00 1.00	48.15 48.15
	45	С	LEU C	9	11.124	31.922	33.685	1.00	76.39
50	46	0	LEU C	9	11.321	31.262	34.690	1.00	76.39
20	47 48	N CA	ASN C	10	10.380	31.476	32.687	1.00	56.03
	49	CB	ASN C ASN C	10 10	9.756	30.161	32.739	1.00	56.03
	50	CG	ASN C	10	8.459 7.912	30.216 28.844	33.531 33.807	1.00	97.06
	51	OD1	ASN C	10	8.527	28.062	34.532	1.00 1.00	97.06 97.06
55	52	ND2	ASN C	10	6.764	28.528	33.218	1.00	97.06
	53	C	ASN C	10	9.460	29.670	31.333	1.00	56.03
	54 55	O N	ASN C PRO C	10	8.594	30.226	30.649	1.00	56.03
	56	CD	PRO C	11 11	10.173 10. 02 2	28.619	30.873	1.00	62.47
60	57	CA	PRO C	11	11.225	28.168 27.865	29.482 31.546	1.00	141.22
	58	CB	PRO C	11	11.726	26.936	30.444	1.00 1.00	62.47 141.22
	59	CG	PRO C	11	10.542	26.774	29.564	1.00	141.22
	60	C	PRO C	11	12.362	28.734	32.097	1.00	62.47
65	61 62	0 N	PRO C PRO C	11	12.512	29.887	31.703	1.00	62.47
	63	CD	PRO C	12 12	13.197 13.127	28.186 26.826	33.000	1.00	68.33
	64	CA	PRO C	12	14.315	28.913	33.565 33.606	1.00	71.60
			-			201010	55.000	1.00	68.33

	65 66	CB CG	PRO C	12 12	· 14.839 13.707	27.958 27.044	34.664 34.925	1.00 1.00	71.60 71.60
	67	С	PRO C	12	15.383	29.190	32.567	1.00	68.33
5	68 ·	0 '	PRO C	12	16.176	30.127	32.696	1.00	68.33
J	69 70	N CA	TRP C	13	15.395	28.352	31.538	1.00	58.74
	71	CB	TRP C	13 13	16.378 16.076	28.444 27.401	30.466 29.401	1.00	58.74
	72	CG	TRP C	13	15.812	26.077	29.969	1.00 1.00	68.19
	73	CD2	TRP C	13	16.476	25.473	31.064	1.00	68.19 68.19
10	74	CE2	TRP C	13	15.848	24.241	31.307	1.00	68.19
	75	CE3	TRP C	13	17.547	25.852	31.873	1.00	68.19
	76 77	CD1 NE1	TRP C	13	14.844	25.220	29.588	1.00	68.19
	78	CZ2	TRP C	13 13	14.848 16.252	24.114 23.380	30.391 32.324	1.00	68.19
15	79	CZ3	TRP C	13	17.950	24.993	32.892	1.00 1.00	68.19
	80	CH2	TRP C	13	17.300	23.771	33.107	1.00	68.19 68.19
	81	C	TRP C	13	16.409	29.810	29.826	1.00	58.74
	82	0	TRP C	13	15.409	30.264	29.288	1.00	58.74
20	83 84	N CA	ASN C ASN C	14	17.570	30.454	29.879	1.00	57.67
20	85	CB	ASN C	14 14	17.729 18.371	31.775 32.746	29.295	1.00	57.67
	86	ČĞ	ASN C	14	19.809	32.414	30.304 30.614	1.00 1.00	148.07
	87	OD1	ASN C	14	20.127	31.304	31.041	1.00	148.07 148.07
~ ~	88	ND2	ASN C	14	20.692	33.383	30.408	1.00	148.07
25	89	Č	ASN C	14	18.508	31.761	27.990	1.00	57.67
	90	0	ASN C	14	18.992	32.785	27.550	1.00	57.67
	91 92	N CA	ARG C ARG C	15	18.645	30.590	27.378	1.00	58.44
	93	CB	ARG C	15 15	19.311 20.634	30.455 29.728	26.078	1.00	58.44
30	94	CG	ARG C	15	21.469	30.131	26.174 27.329	1.00 1.00	68.23
	95	CD	ARG C	15	22.779	29,404	27.261	1.00	68.23 68.23
	96	NE	ARG C	15	23.607	29.885	26.172	1.00	68.23
	97	CZ	ARG C	15	24.492	29.119	25.560	1.00	68.23
35	98 99	NH1	ARG C	15	24.614	27.865	25.950	1.00	68.23
33	100	NH2 C	ARG C	15	25.267 18.345	29.599	24.589	1.00	68.23
	101	ŏ	ARG C	15 15	18.206	29.540 28.379	25.394 25.805	1.00	58.44
	102	Ň	ILE C	16	17.648	30.048	24.386	1.00 1.00	58.44 56.07
40	103	CA	ILE C	16	16.691	29.214	23.693	1.00	56.07
40	104	CB	ILE C	16	15.279	29.668	23.944	1.00	49.05
	105	CG2	ILE C	16	14.939	29.490	25.385	1.00	49.05
	106 107	CG1 CD1	ILE C	16	15.128	31.116	23.520	1.00	49.05
	108	C	ILE C	16 16	13.760 16.889	31.675 29.154	23.801	1.00	49.05
45	109	ŏ	ILE C	16	17.607	29.956	22.201 21.610	1.00 1.00	56.07
	110	Ň	PHE C	17	16.221	28.178	21.608	1.00	56.07 80.97
	111	CA	PHE C	17	16.247	27.906	20.188	1.00	80.97
	112	CB	PHE C	17	15.846	26.458	19.984	1.00	52.57
50	113	CG	PHE C	17	16.996	25.503	19.972	1.00	52.57
50	114 115	CD1 CD2	PHE C	17 17	16.878	24.248	20.554	1.00	52.57
	116	CE1	PHE C	17	18.173 17.897	25.830 23.329	19.278 20.455	1.00	52.57
	117	CE2	PHE C	17	19.207	24.912	19.167	1.00 1.00	52.57 52.57
~ ~	118	CZ	PHE C	17	19.063	23.648	19.759	1.00	52.57
55	119	C	PHE C	17	15.251	28.793	19.468	1.00	80.97
	120 121	0	PHE C	17	14.320	29.320	20.074	1.00	80.97
	122	N CA	LYS C Lys C	18	15.429	28.937	18.161	1.00	59.00
	123	CB	LYS C	18 18	14.529 15.065	29.761 29.846	17.349 15.921	1.00	59.00
60	124	ČĞ	LYS C	18	14.313	30.790	15.003	1.00 1.00	195.91 195.91
	125	CD	LYS C	18	15.142	31.059	13.761	1.00	195.91
	126	CE	LYS C	18	14.441	32.000	12.803	1.00	195.91
	127	NZ	LYS C	18	13.160	31.413	12.321	1.00	195.91
65	128 129	C	LYS C	18	13.123	29.162	17.349	1.00	59.00
J J	130	N	LYS C GLY C	18	12.937	27.974	17.129	1.00	59.00
	131	CA	GLY C	19 19	12.122 10,774	29.973 29.457	17.630 17.592	1.00	76.33
	132	Č	GLY C	19	10.178	28.991	17.582 18.886	1.00 1.00	76.33 76.33
70	133	0	GLY C	19	8.971	28.747	18.970	1.00	76.33 76.33
70	134	N	GLU C	20	10.998	28.857	19.916	1.00	72.26

	135 136	CA CB	GLU C	20 20	-10.460 11.590	28.427 27.847	21.211	1.00	72.26
	137	CG	GLU C	20	12,410	26.815	22.059 21.296	1.00 1.00	102.87
_	138	CD	. GLU C	20	13.457	26.129	22.152	1.00	102.87 102.87
5	139	OE1	GLU C	20	14.291	26.830	22.758	1.00	102.87
	140 141	OE2 C	GLU C	20	13.452	24.884	22.210	1.00	102.87
	142	ŏ	GLU C	20 20	9.739 9.803	29.579 30.730	21.956	1.00	72.26
	143	Ň	ASN C	21	9.030	29.264	21.525 23.040	1.00 1.00	72.26
10	144	CA	ASN C	21	8.336	30.295	23.787	1.00	57.87 57.87
	145	CB	ASN C	21	6.839	30.041	23.853	1.00	107.77
	146	CG	ASN C	21	6.273	29.544	22.563	1.00	107.77
	147 148	OD1 ND2	ASN C ASN C	21	6.639	30.019	21.477	1.00	107.77
15	149	C	ASN C	21 21	5.353 8.841	28.591 30.401	22.690 25.220	1.00	107.77
	150	Ö	ASN C	21	9.136	29.391	25.859	1.00 1.00	57.87 57.87
	151	N	VAL C	22	8.921	31.625	25.735	1.00	64.18
	152	CA	VAL C	22	9.364	31.858	27.099	1.00	64.18
20	153 154	CB CG1	VAL C	22	10.797	32.278	27.139	1.00	42.75
20	155	CG2	VAL C VAL C	22 22	10.981 11.231	33.583	26.376	1.00	42.75
	156	C	VAL C	22	8.542	32.452 32.997	28.585 27.677	1.00	42.75
•	157	ŏ	VAL C	22	8.115	33.897	26.936	1.00 1.00	64.18
0.5	158	N	THR C	23	8.347	32.977	28.998	1.00	64.18 75.81
25	159	CA	THR C	23	7.534	33.987	29.693	1.00	75.81
	160	CB	THR C	23	6.369	33.301	30.399	1.00	170.16
	161 162	OG1 CG2	THR C	23	5.651	32.492	29.459	1.00	170.16
	163	C	THR C THR C	23 23	5.442 8.328	34.327	31.005	1.00	170.16
30	164	ŏ	THR C	23	8.978	34.776 34.183	30.730	1.00	75.81
	165	N	LEU C	24	8.292	36.101	31.572 30.684	1.00 1.00	75.81
	166	CA	LEU C	24	9.071	36.861	31.656	1.00	82.13 82.13
	167	CB	LEU C	24	9.899	37.962	30.995	1.00	55.82
35	168	CG	LEU C	24	10.586	37.719	29.653	1.00	55.82
55	169 170	CD1 CD2	LEU C	24	11.621	38.790	29.358	1.00	55.82
	171	C	LEU C	24 24	11.241 8.182	36.405	29.664	1.00	55.82
	172	ŏ	LEU C	24	7.526	37.506 38.505	32.677 32.391	1.00 1.00	82.13
	173	N	THR C	25	8.184	36.967	33.888	1.00	82.13 46.04
40	174	CA	THR C	25	7.333	37.517	34.921	1.00	46.04
	175	CB	THR C	25	6.859	36.406	35.852	1.00	88.77
	176 177	OG1 CG2	THR C	25	6.235	35.384	35.064	1.00	88.77
	178	C	THR C THR C	25 25	5.846	36.939	36.851	1.00	88.77
45	179	ŏ	THR C	25 25	8.047 9.225	38.614 38.493	35.693 36.009	1.00	46.04
	180	Ň	CYS C	26	7.360	39.719	35.962	1.00 1.00	46.04 99.22
	181	CA	CYS C	26	7.988	40.779	36.730	1.00	99.22
	182	C	CYS C	26	7.833	40.454	38.201	1.00	99.22
50	183 184	0	CYS C	26	6.787	39.984	38.644	1.00	99.22
50	185	CB SG	CYS C	26	7.353	42.132	36.440	1.00	145.11
	186	N	ASN C	26 27	8.267 8.897	43.513 40.697	37.198	1.00	145.11
	187	ĊA	ASN C	27	8.936	40 404	38.944	1.00	197.95
	188	СВ	ASN C	27	9.427	40.461 41.723	40.370 41.048	1.00 1.00	197.95 249.36
55	189	CG	ASN C	27	9.841	41.459	42.424	1.00	249.36
	190	OD1	ASN C	27	10.558	40.419	42.666	1.00	249.36
	191 192	ND2	ASN C	27	9.710	42.399	43.346	1.00	249.36
	193	CO	ASN C ASN C	27	7.618	40.026	41.003	1.00	197.95
60 .	194	Ň	GLY C	27 28	6.829 7.392	40.859 38.719	41.440	1.00	197.95
	195	CA	GLY C	28	6.162	38.203	41.065 41.644	1.00 1.00	214.74
	196	Ç	GLY C	28	6.121	36.711	41.398	1.00	214.74 214.74
	197	0	GLY C	28	6.177	38.27 6	40.255	1.00	214.74
65	198	N	ASN C	29	6.006	35.922	42.456	1.00	249.28
UJ	199 200	CA CB	ASN C	29	6.011	34.476	42.322	1.00	249.28
	201	CG	ASN C ASN C	29 20	6.332 6.655	33.825	43.676	1.00	216.11
	202	OD1	ASN C	29 29	6.655 6.877	32.353 31.849	43.552 42.450	1.00	216.11
	203	ND2	ASN C	29	6.701	31.657	42.450 44.681	1.00 1.00	216.11
70	204	С	ASN C	29	4.731	33.880	41.751	1.00	216.11 249.28

	205 206 207	O N CA	ASN C ASN C ASN C	29 30 30	- 4.781 3.584 2.325	33.119 34.225 33.663	40.788 42.328 41.851	1.00 1.00	249.28 235.48
5	208 209 210	CB CG OD1	ASN C ASN C ASN C	30 30 30	1.763 2.660 3.006	32.685 31.487 31.152	42.889 43.106	1.00 1.00 1.00	235.48 219.86 219.86
	211 212 213	ND2 C	ASN C ASN C ASN C	30 30	3.040 1.251	30.831 34.682	44.240 42.019 41.498	1.00 1.00 1.00	219.86 219.86 235.48
10	214 215 216	N CA CB	PHE C PHE C PHE C	30 31 31	0.931 0.690 -0.373	34.878 35.329 36.291	40.325 42.515 42.280	1.00 1.00 1.00	235.48 241.86 241.86
15	217 218 219	CG CD1 CD2	PHE C PHE C PHE C	31 31 31	-1.597 -2.076 -1.432	35.920 34.504 33.431	43.123 42.908 43.523	1.00 1.00 1.00	249.47 249.47 249.47
	220 221 222	CE1 CE2 CZ	PHE C PHE C PHE C	31 31 31 31	-3.154 -1.858 -3.588	34.240 32.115 32.927	42.066 43.307 41.843	1.00 1.00 1.00	249.47 249.47 249.47
20	223 224 225	C O N	PHE C PHE C PHE C	31 31 32	-2.936 0.022 0.520	31.863 37.743 38.109	42.463 42.516 43.587	1.00 1.00 1.00	249.47 241.86 241.86
	226 227 228	CA CB CG	PHE C PHE C PHE C	32 32 32 32	-0.212 0.108 1.132 1.755	38.559 39.985 40.302	41.489 41.512 40.423	1.00 1.00 1.00	249.62 249.62 249.66
25	229 230 231	CD1 CD2 CE1	PHE C PHE C PHE C	32 32 32 32	2.582 1.510 3.147	41.655 41.907 42.675	40.560 41.614 39.643	1.00 1.00 1.00	249.66 249.66 249.66
30	232 233 234	CE2 CZ C	PHE C PHE C PHE C	32 32 32 32	2.093 2.900 -1.151	43.108 43.918 44.146	41.753 39.791 40.828	1.00 1.00 1.00	249.66 249.66 249.66
	235 236 237	O N CA	PHE C GLU C GLU C	32 33 33	-2.197 -1.054 -2,224	40.815 40.259 42.139 42.994	41.269 40.930 41.416	1.00 1.00 1.00	249.62 249.62 249.77
35	238 239 240	CB CG CD	GLN C GLN C GLN C	33 33 33	-2.704 -4.023 -5.159	42.994 43.604 44.344 43.406	41.200 42.503 42.358	1.00 1.00 1.00	249.77 249.65 249.65
	241 242 243	OE1 OE2 C	GLU C GLU C GLU C	33 33 33	-5.159 -6.051 -2.110	43.406 42.298 43.779 44.128	42.025 42.562 41.239	1.00 1.00 1.00	249.65 249.65 249.65
40	244 245 246	O N CA	GLU C VAL C VAL C	33 34 34	-2.952 -1.107 -0.949	44.257 44.982 46.113	40.194 39.301 40.365	1.00 1.00 1.00	249.77 249.77 243.09
45	247 248 249	CB CG1 CG2	VAL C VAL C VAL C	34 34 34	0.351 0.508 0.302	46.880 48.060 47.386	39.471 39.775 38.826 41.184	1.00 1.00 1.00	243.09 249.25 249.25
	250 251 252	C O N	VAL C VAL C SER C	34 34 35	-0.990 -0.603 -1.494	45.721 44.616 46.644	38.002 37.615 37.196	1.00 1.00 1.00	249.25 243.09 243.09
50	253 254 255	CA CB OG	SER C SER C SER C	35 35 35	-1.605 -3.021 -3.296	46.453 46.778 48.166	35.764 35.290 35.411	1.00 1.00 1.00	146.24 146.24 174.88
	256 257 258	C O N	SER C SER C SER C	35 35 36	-0.617 -0.518 0.095	47.400 47.438 48.179	35.103 33.878 35.919	1.00 1.00 1.00 1.00	174.83 148.24 146.21
55	259 260 261	CA CB OG	SER C SER C SER C	36 36 36	1.091 0.986 1.420	49.114 50.475 50.408	35.408 36.105 37.452	1.00 1.00 1.00	112.51 112.51 242.80 242.80
60	262 263 264	C O N	SER C SER C THR C	36 36 37	2.486 3.088 2.985	48.535 48.707 47.834	35.635 36.700 34.620	1.00 1.00 1.00	112.51 112.51 147.41
	265 266 267	CA CB OG1	THR C THR C THR C	37 37 37	4.301 4.185 3.393	47.220 45.679 45.242	34.655 34.635 35.748	1.00 1.00 1.00	147.41 242.04 242.04
65	268 269 270	CG2 C O	THR C THR C THR C	37 37 37	5.553 5.004 4.382	45.039 47.708 47.834	34.720 33.399 32.345	1.00 1.00 1.00	242.04 147.41 147.41
70	271 272 273	N CA CB	LYS C LYS C LYS C	38 38 38	6.289 7.046 7.794	48.009 48.490 49.755	33.512 32.361 32.733	1.00 1.00 1.00	114.65 114.65 121.59
70	274	CG	LYS C	38	6.890	50.832	33.262	1.00	121.59

	275	CD	LYS C	38	· 7.679	52.074	33.632	1.00	121.59
	276	CE	LYS C	38	6.757	53.183	34.088	1.00	121.59
	277	NZ	LYS C	38	7.518	54.413	34.415	1.00	121.59
5	278	C	· LYS C	38	8.045	47.459	31.856	1.00	114.65
)	279	0	LYS C	38	8.640	46.745	32.652	1.00	114.65
	280	N	TRP C	39	8.222	47.373	30.538	1.00	83.37
	281 282	CA CB	TRP C	39	9.182	46.434	29.954	1.00	83,37
	283	CG	TRP C	39 39	8.477	45.308	29.202	1.00	59.20
10	284	CD2	TRP C	39	7.651 8.116	44.439 43.493	30.060	1.00	59.20
	285	CE2	TRP C	39	6.973	43.493 42.881	31.026	1.00	59.20
	286	CE3	TRP C	39	9.391	43.100	31.590 31.474	1.00	59.20
	287	CD1	TRP C	39	6.298	44.369	30.071	1.00 1.00	59.20
	288	NE1	TRP C	39	5.881	43.435	30.990	1.00	59.20
15	289	CZ2	TRP C	39	7.061	41.892	32.576	1.00	59.20 59.20
	290	CZ3	TRP C	39	9.476	42.119	32.456	1.00	59.20
	291	CH2	TRP C	39	8.312	41.524	32.998	1.00	59.20
	292	C	TRP C	39	10.086	47.179	28.990	1.00	83.37
20	293	0	TRP C	39	9.612	47.932	28.144	1.00	83.37
20	294 295	N CA	PHE C PHE C	40	11.387	46.963	29.116	1.00	81.86
	296	CB	PHE C	40 40	12.330	47.639	28.248	1.00	81.86
	297	CG	PHE C	40	13.204 12.433	48.591	29.062	1.00	132.74
	298	CD1	PHE C	40	11.846	49.601 49.258	29.852 31.063	1.00	132.74
25	299	CD2	PHE C	40	12.305	50.903	29.393	1.00 1.00	132.74
	300	CE1	PHE C	40	11.141	50.201	31.812	1.00	132.74 132.74
	301	CE2	PHE C	40	11.603	51.853	30.130	1.00	132.74
	302	CZ	PHE C	40	11.020	51.501	31.344	1.00	132.74
20	303	С	PHE C	40	13.225	46.677	27.474	1.00	81.86
30	304	0	PHE C	40	14.321	46.333	27.917	1.00	81.86
	305	N	HIS C	41	12.761	46.239	26.314	1.00	70.61
	306 307	CA	HIS C	41	13.552	45.334	25.490	1.00	70.61
	307 308	CB CG	HIS C	41	12.633	44.671	24.470	1.00	75.99
35	309	CD2	HIS C HIS C	41 41	13.339	43.759	23.528	1.00	75.99
-	310	ND1	HIS C	41	13.192 14.327	43.567 42.893	22.198	1.00	75.99
	311	CE1	HIS C	41	14.765	42.207	23.933 22.892	1.00 1.00	75.99
	312	NE2	HIS C	41	14.093	42.598	21.826	1.00	75.99 75.99
	313	С	HIS C	41	14.671	46.118	24.794	1.00	70.61
40	314	0	HIS C	41	14.408	46.922	23.918	1.00	70.61
	315	N	ASN C	42	15.916	45.879	25.177	1.00	90.99
	316	CA	ASN C	42	17.063	46.600	24.615	1.00	90.99
	317	CB	ASN C	42	17.150	46.463	23.085	1.00	90.93
45	318 319	CG OD1	ASN C ASN C	42	17.611	45.087	22.641	1.00	90.93
43	320	ND2	ASN C	42 42	17.149	44.097	23.186	1.00	90.93
	321	C	ASN C	42	18.495 16.966	45.007 48.077	21.649	1.00	90.93
	322	ŏ	ASN C	42	17.474	48.926	24.971 24.246	1.00	90.99
	323	Ň	GLY C	43	16.315	48.394	26.086	1.00 1.00	90.99
50	324	CA	GLY C	43	16.177	49.792	26.478	1.00	101.51 101.51
	325	С	GLY C	43	9. ت.14	50.456	25.997	1.00	101.51
	326	0	GLY C	43	14.265	51.235	26.721	1.00	101.51
	327	N	SER C	44	14.492	50.140	24.769	1.00	159.89
55	328	CA	SER C	44	13.276	50.686	24.182	1.00	159.89
22	329 330	CB	SER C	44	13.183	50.282	22.705	1.00	153,29
	331	og	SER C SER C	44	14.375	50.612	22.007	1.00	153.29
	332	C	SER C	44 44	12.046 11.886	50.168	24.931	1.00	159.89
	333	Ň	LEU C	45	11.179	48.962 51.076	25.114	1.00	159.89
60	334	CA	LEU C	45	9.969	50.682	25.368 26.091	1.00	127.30
	335	СВ	LEU C	45	9.143	51.925	26.443	1.00 1.00	127.30
	336	CG	LEU C	45	7.855	51.691	27.238	1.00	113.27 113.27
	337	CD1	LEU C	45	8.167	50.902	28.502	1.00	113.27
CF	338	CD2	LEU C	45	7.210	53.024	27.593	1.00	113.27
65	339	C	LEU C	45	9.126	49.705	25.261	1.00	127.30
	340	0	LEU C	45	9.084	49.805	24.039	1.00	127.30
	341	N CA	SER C	46	8.458	48.758	25.915	1.00	104.59
	342	CA	SER C	46	7.636	47.784	25.206	1.00	104.59
70	343 344	CB OG	SER C	46 46	7.802	46.400	25.829	1.00	120.90
. •		OG	SER C	46	7.052	45.423	25.111	1.00	120.90

	345	C	SER C	46	- 6.194	48.226	25.309	1.00	104.59
	346	0	SER C	46	5.867	49.072	26.127	1.00	104.59
	347	Ņ	GLU C	47	5.320	47.643	24.495	1.00	161.06
5	348	CA	GLU C	47	3.919	48.057	24.551	1.00	161.06
2	349	CB	GLU C	47	3.295	48.100	23.152	1.00	249.30
	350	CG	GLU C	47	4.218	48.523	22.010	1.00	249.30
	351	CD	GLU C	47	3.700	48.108	20.617	1.00	249.30
	352	OE1	GLU C	47	4.006	46.969	20.155	1.00	249.30
10	353 354	OE2	GLU C	47	2.988	48.918	19.972	1.00	249.30
10	355	CO	GLU C	47	3.070	47.171	25.505	1.00	161.06
	356	N		47	1.875	47.409	25.648	1.00	161.06
	357	CA	GLU C	48	3.655	46.147	26.142	1.00	104.22
	358	CB	GLU C	48 48	2.859	45.337	27.077	1.00	104.22
15	359	CG	GLU C	48	3.427 2.742	43.913	27.044	1.00	144.62
	360	CD	GLU C	48	1.288	43.070 42.704	28.349	1.00	144.62
	361	. OE1	GLU C	48	1.034	41.897	28.064	1.00	144.62
	362	OE2	GLU C	48	0.396	43.221	27.140 28.775	1.00	144.62
	363	C	GLU C	48	2.829	46.060	28.424	1.00	144.62
20	364	0	GLU C	48	3.708	46 368	28.724	1.00 1.00	104.22
	365	N	THR C	49	1.813	40.771	29.229	1.00	104.22
	366	CA	THR C	49	1.677	46.399	30.529	1.00	87.76
	367	CB	THR C	49	0.505	47.406	30.547	1.00	87.76
0.5	368	OG1	THR C	49	-0.713	46.751	30.168	1.00	167.47
25	369	CG2	THR C	49	0.788	48.546	29.576	1.00	167.47
	370	С	THR C	49	1.461	45.342	31.601	1.00	167.47 87.76
	371	0	THR C	49	1.832	45.537	32.751	1.00	87.76
	372	N	ASN C	50	0.872	44.210	31.227	1.00	92.41
20	373	CA	ASN C	50	0.637	43.123	32.180	1.00	92.41
30	374	СВ	ASN C	50	0.006	41.921	31.455	1.00	211.05
	375	CG	ASN C	50	-0.583	40.901	32.411	1.00	211.05
	376	OD1	ASN C	50	-0.245	40.896	33.593	1.00	211.05
	377	ND2	ASN C	50	-1.449	40.025	31.907	1.00	211.05
35	378	Ç	ASN C	50	2.006	42.743	32.772	1.00	92.41
22	379	0	ASN C	50	3.035	42.908	32.125	1.00	92.41
	380	N	SER C	51	2.026	42.252	34.005	1.00	91.81
	381	CA	SER C	51	3.280	41.858	34.640	1.00	91.81
	382	CB	SER C	51	3.042	41.518	36.117	1.00	188.83
40	383 384	og	SER C	51	2.293	40.322	36.271	1.00	188.83
70	385	C	SER C	51	3.948	40.661	33.944	1.00	91.81
	386	O N	SER C	51	5.130	40.414	34.137	1.00	91.81
	387	CA CA	SER C SER C	52	3.199	39.919	33.136	1.00	82.66
	388	CB	SER C	52 52	3.750	38.764	32.450	1.00	82.66
45	389	ÖĞ	SER C	52 52	2.862	37.530	32.662	1.00	107.08
	390	č	SER C	52 52	2.845 3.860	37.147	34.025	1.00	107.08
	391	ŏ	SER C	52 52	2.866	39.064	30.976	1.00	82.66
	392	Ň	LEU C	53	5.089	39.155 39.228	30.271	1.00	82.66
	393	CA	LEU C	53	5.386	39.501	30.524 29.126	1.00	52.71
50	394	CB	LEU C	53	6.563	40.483	29.036	1.00	52.71
	395	CG	LEU C	53	7.380	40.539	27.742	1.00	59.51
	396	CD1	LEU C	53	6.474	40.524	26.514	1.00 1.00	59.51
	397	CD2	LEU C	53	8.217	41.797	00-		59.51 50.51
	398	C	LEU C	53	5.741	38.215	27.765 28.378	1.00 1.00	59.51
55	399	0	LEU C	53	6.880	37.750	28.462	1.00	52.71 52.71
	400	N	ASN C	54	4.794	37.650	27.631	1.00	78.83
	401	CA	ASN C	54	5.073	36.425	26.889	1.00	78.83
	402	CB	ASN C	54	3.777	35.731	26.511	1.00	114.28
60	403	CG	ASN C	54	3.093	35.117	27.699	1.00	114.28
60	404	OD1	ASN C	54	3.685	34.315	28.415	1.00	114.28
	405	ND2	ASN C	54	1.842	35.488	27.922	1.00	114.28
	406	Ç	ASN C	54	5.898	36.641	25.629	1.00	78.83
	407	0	ASN C	54	5.983	37.745	25.099	1.00	78.83
65	408	N	ILE C	55	6.527	35.566	25.174	1.00	69.41
O)	409	CA	ILE C	55	7.321	35.571	23.962	1.00	69.41
	410	CB	ILE C	55	8.814	35.555	24.270	1.00	55.40
•	411	CG2	ILE C	55	9.596	35.167	23.036	1.00	55.40
	412	CG1	ILE C	55	9.238	36.952	24.724	1.00	55.40
70	413	CD1	ILE C	55	10.730	37.122	25.012	1.00	55.40
,,	414	С	ILE C	55	6.935	34.320	23.210	1.00	69.41

	415	0	ILE C		. 7 040	00.000			
	416	Ň	VAL C	55 56	· 7.048 6.442	33 <i>.2</i> 32 34.473	23.744	1.00	69.41
	417	ĈA	VAL C	56	6.046	33.317	21.989 21.199	1.00	107.00
_	418	CB .	VAL C	56	4.721	33.566	20.504	1.00 1.00	107.00
5	419	CG1	VAL C	56	4.126	32.254	20.058	1.00	128.23 128.23
	420	CG2	VAL C	56	3.772	34.277	21.453	1.00	128.23
	421	C	VAL C	56	7.132	33.041	20.171	1.00	107.00
	422	0	VAL C	56	8.236	33.546	20.317	1.00	107.00
10	423 424	N CA	ASN C ASN C	57	6.837	32.251	19.142	1.00	99.37
10	425	CB	ASN C ASN C	57 57	7.833	31.906	18.123	1.00	99.37
	426	CG	ASN C	57	7.201 6.217	31.916 30.781	16.733	1.00	170.52
	427	OD1	ASN C	57	6.543	29.617	16.541 16.766	1.00	170.52
	428	ND2	ASN C	57	5.000	31.115	16.127	1.00 1.00	170.52 170.52
15	429	С	ASN C	57	9.053	32.828	18.157	1.00	99.37
	430	0	ASN C	57	9.105	33.850	17.480	1.00	99.37
	431	N.	ALA C	58	10.033	32.443	18.966	1.00	78.85
	432	CA	ALA C	58	11.241	33.220	19.162	1.00	78.85
20	433 434	CB C	ALA C ALA C	58	12.180	32.478	20.085	1.00	109.58
20	435	Ö	ALA C	58 58	11.951	33.558	17.878	1.00	78.85
	436	Ň	LYS C	59	12.358 12.094	32.681 34.845	17.139	1.00	78.85
	437	CA	LYS C	59	12.812	35.317	17.610 16.428	1.00 1.00	66.66
	438	CB	LYS C	59	11.988	36.405	15.726	1.00	66.66 201.62
25	439	CG	LYS C	59	10.597	35.939	15.295	1.00	201.62
	440	CD	LYS C	59	9.751	37.07 0	14.724	1.00	201.62
	441	CE	LYS C	59	8.374	36.569	14.307	1.00	201.62
	442 443	NZ	LYS C	59	7.518	37.663	13.775	1.00	201.62
30	444	C	LYS C LYS C	59	14.146	35. 8 90	16.953	1.00	66.66
50	445	Ň	PHE C	59 60	14.194 15.224	36.455 35.743	18.055	1.00	66.66
	446	CA	PHE C	60	16.515	36.265	16.188 16.616	1.00 1.00	69.57
	447	CB	PHE C	60	17.455	36.314	15.438	1.00	69.57 112.86
25	448	CG	PHE C	60	17.775	34.974	14.896	1.00	112.86
35	449	CD1	PHE C	60	18.097	34.805	13.562	1.00	112.86
	450	CD2	PHE C	60	17.757	33.867	15.718	1.00	112.86
	451 452	· CE1 CE2	PHE C PHE C	60	18.396	33.553	13.046	1.00	112.86
	453	CZ	PHE C	60 60	18.050 18.372	32.608 32.452	15.217	1.00	112.86
40 .	454	č	PHE C	60	16.436	37.644	13.877 17.258	1.00 1.00	112.86
	455	ŏ	PHE C	60	17.213	37.958	18.172	1.00	69.57 69.57
	456	N	GLU. C	61	15.498	38.466	16.785	1.00	114.60
	457	CA	GLU C	61	15.308	39.823	17.303	1.00	114.60
45	458	CB	GLU C	61	14.268	40.583	16.482	1.00	179.88
43	459 460	CG	GLU C	61	14.629	. 40.775	15.025	1.00	179.88
	461	CD OE1	GLU C GLU C	61	14.804	39.464	14.296	1.00	179.88
	462	OE2	GLU C	61 61	13.874 15.871	38.631 39.269	14.334	1.00	179.88
	463	c	GLU C	61	14.865	39.831	13.682 18.757	1.00 1.00	179.88
50	464	O	GLU C	61	15.064	40.828	19.451	1.00	114.60 114.60
	465	N	ASP C	62	14.251	38.737	19.214	1.00	61.26
	466	CA	ASP C	62	13.807	38.654	20.605	1.00	61.26
	467	CB	ASP C	62	12.884	37.457	20.801	1.00	109.78
55	468 469	CG OD1	ASP C	62	11.707	37.472	19.842	1.00	109.78
33	470	OD2	ASP C	62 62	11.182	38.574	19.564	1.00	109.78
	471	C	ASP C	62	11.296 15.018	36.385 38.559	19.374	1.00	109.78
	472	Ö	ASP C	62	14.915	38.859	21.542 22.726	1.00 1.00	61.26
	473	N	SER C	63	16.166	38.159	20.999	1.00	61.26 49.60
60	474	CA	SER C	63	17.390	38.050	21.776	1.00	49.60
	475	CB	SER C	63	18.539	37.599	20.873	1.00	59.31
	476	og .	SER C	63	18.360	36.265	20.405	1.00	59.31
	477 478	C O	SER C	63	17.669	39.432	22.294	1.00	49.60
65	479	N	SER C GLY C	63 64	17.647	40.359	21.520	1.00	49.60
	480	CA	GLY C	64	17.918 18.192	39,595 40,936	23.583	1.00	66.63
	481	Ċ	GLY C	64	18.223	41.119	24.070 25.579	1.00 1.00	66.63
	482	0	GLY C	64	18.210	40.154	26.339	1.00	66.63 68.63
70	483	N _.	GLU C	65	18.288	42.371	26.018	1.00	55.08
70	484	CA	GLU C	65	18.306	42.725	27.440	1.00	55.08

	485	СВ	GLU C	65	- 19.339	43.828	27.632	1.00	150 40
	486	CG	GLU C	65	19.349	44.480	28.979	1.00	156.42 156.42
	487	CD	GLU C	65	20.163	45.756	28.978	1.00	156.42
5	488 . 489	OE1 · OE2	GLU C	65 65	19.785	46.700	28.254	1.00	156.42
3	490	C	GLU C	65 65	21.183 16.899	45.817 43.218	29.696 27.844	1.00	156.42
	491	ŏ	GLU C	65	16.346	44.123	27.8 44 27.213	1.00 1.00	55.08
	492	N	TYR C	66	16.307	42.625	28.871	1.00	55.08 61.99
10	493	CA	TYR C	66	14.981	43.056	29.291	1.00	61.99
10	494 495	CB	TYR C	66	14.013	41.901	29.181	1.00	58.17
	495 496	CG CD1	TYR C TYR C	66 66	13.740	41.415	27.806	1.00	58.17
	497	CE1	TYR C	66	14.658 14.365	40.634 40.112	27.133 25.886	1.00 1.00	58.17
	498	CD2	TYR C	66	12.520	41.681	27.198	1.00	58.17 58.17
15	499	CE2	TYR C	66	12.213	41.170	25.953	1.00	58.17
	500	CZ	TYR C	66	13.134	40.379	25.300	1.00	58.17
	501 502	OH C	TYR C TYR C	66 66	12.786 14.950	39.826	24.081	1.00	58.17
	503	ŏ	TYR C	66	15.850	43.525 43.192	30.746 31.522	1.00 1.00	61.99
20	504	N	LYS C	67	13.899	44.254	31.132	1.00	61.99 84.17
	505	CA	LYS C	67	13.751	44.703	32.516	1.00	84.17
	506	CB	LYS C	67	14.789	45.766	32.837	1.00	116.03
	507 508	. CO	LYS C LYS C	67 67	14.858	46.850	31.807	1.00	116.03
25	509	CE	LYS C	67	15.986 16.177	47.803 48.787	32.118 30.983	1.00 1.00	116.03
	510	NZ	LYS C	67	17.324	49.693	31.252	1.00	116.03 116.03
	511	Ç	LYS C	67	12.369	45.249	32.762	1.00	84.17
	512	0	LYS C	67	11.696	45.655	31.819	1.00	84.17
30	513 514	N CA	CYS C CYS C	68	11.933	45.229	34.020	1.00	81.35
50	515	Ĉ	CYS C	68 68	10.624 10.749	45.780 46.788	34.350 35.467	1.00	81.35
	516	ō	CYS C	68	11.761	46.811	36.145	1.00 1.00	81.35 81.35
	517	CB	CYS C	68	9.619	44.672	34.717	1.00	117.98
35	518	SG	CYS C	68	9.997	43.610	36.128	1.00	117.98
33	519 520	N CA	GLN C GLN C	69	9.734	47.628	35.627	1.00	106.08
	520 521	CB	GLN C	69 69	9. 722 10.471	48.638 49.900	36.664	1.00	106.08
	522	ČĠ	GLN C	69	10.166	51.173	36.188 36.978	1.00 1.00	124.18 124.18
40	523	CD	GLN C	69	10.841	52.407	36.397	1.00	124.18
40	524	OE1	GLN C	69	10.720	52.687	35.205	1.00	124.18
	525 526	NE2 C	GLN C	69	11.542	53.160	37.244	1.00	124.18
	527	ŏ	GLN C GLN C	69 69	8.265 7.416	48.974 48.787	36.930 36.054	1.00	106.08
	528	Ň	HIS C	70	7.967	49.457	38.131	1.00	106.08 181.43
45	529	CA	HIS C	70	6.609	49.830	38.469	1.00	181.43
	530	СВ	HIS C	70	6.177	49.107	39.764	1.00	144.62
	531 532	CD2	HIS C	70	6.062	47.635	39.606	1.00	144.62
	533	ND1	HIS C HIS C	70 70	6.901 4.972	46.634	39.977	1.00	144.62
50	534	CE1	HIS C	70	5.121	47.041 45.722	39.030 39.060	1.00 1.00	144.62
	535	NE2	HIS C	70	6.283	45.464	39.631	1.00	144.62 144.62
	536	Ç	HIS C	70	6.421	51.335	38.609	1.00	181.43
	537 538	O.	HIS C	70	7.299	52.112	38.268	1.00	181.43
55	539	N CA	GLN C	71 71	5.254 4.925	51.714 53.108	39.108	1.00	249.25
	540	CB	GLN C	71	3.550	53.209	39.290 39.950	1.00 1.00	249.25 249.45
	541	CG	GLN C	71	2.717	54.409	39.544	1.00	249.45
	542	CD	GLN C	71	2.659	54.624	38.057	1.00	249.45
60	543 544	OE1	GLN C	71	1.970	53.886	37.367	1.00	249.45
UU	545	NE2 C	GLN C GLN C	71 71	3.360 5.988	55.626	37.553	1.00	249.45
	546	ŏ	GLN C	71	6.510	53.876 54.891	40.093 39.634	1.00 1.00	249.25 249.25
	547	N	GLN C	72	6.321	53.366	41.276	1.00	190.92
<i>(F</i>	548	CA	GLN C	72	7.312	54.001	42.145	1.00	190.92
65	549	CB	GLN C	72	6.639	54.552	43.406	1.00	249.44
	550 551	CG CD	GLN C	72	7.556	55.342	44.333	1.00	249.44
	552	OE1	GLN C GLN C	72 72	6.833 5.871	55. 90 0 56.656	45.543 45.411	1.00	249.44
	553	NE2	GLN C	72	7.296	55.530	45.411 46.734	1.00 1.00	249.44 249.44
70	554	C	GLN C	72	8.427	53.034	42.546	1.00	190.92
								· -	

	555 556	0 N	GLN C VAL C	72 73	- 8.660 9.118	52.788 52.481	43.734 41.556	1.00 1.00	190.92 211.52
	557	CA	VAL C	73	10.183	51.531	41.836	1.00	211.52
5	558 .	CB	VAL C	73	9.649	50.092	41.803	1.00	215.95
,	559 560	CG1	VAL C	73	10.667	49.148	42.403	1.00	215.95
	560 561	CG2 C	VAL C	73	8.338	50.011	42.539	1.00	215.95
	562	ŏ	VAL C	73 73	11.297 11.053	51.639	40.816	1.00	211.52
	563	Ň	ASN C	74	12.525	51.942 51.391	39.649 41.256	1.00	211.52
10	564	CA	ASN C	74	13.656	51.454	40.349	1.00 1.00	137.61
	565	СВ	ASN C	74	14.950	51.650	41.136	1.00	137.61 154.43
	566	CG	ASN C	74	14.895	52.860	42.037	1.00	154.43
	567	OD1	ASN C	74	14.408	53.920	41.631	1.00	154.43
15	568 569	ND2	ASN C ASN C	74	15.401	52.711	43.259	1.00	154.43
13	570	C O	ASN C	74	13.708	50.169	39.523	1.00	137.61
	571	N	GLU C	74 75	13.641	49.062	40.063	1.00	137.61
	572	CA	GLU C	75 75	13.807 13.862	50.341 49.236	38.205 37.248	1.00	102.99
	573	СВ	GLU C	75	14.305	49.764	35.881	1.00 1.00	102.99
20	574	CG	GLU C	75	15.294	50.916	35.952	1.00	231.35 . 231.35
	575	CD	GLU C	75	15.534	51.559	34.601	1.00	231.35
	576	OE1	GLU C	75	14.547	51.970	33.952	1.00	231.35
	577 578	OE2	GLU C	75	16.710	51.657	34,190	1.00	231.35
25	579	c o	GLU C	75 75	14.749	48.080	37.693	1.00	102.99
	580	Ň	SER C	75 76	15.794 14.305	48.281	38.296	1.00	102.99
	581	ĊA	SER C	76	14.987	46.868 45. 62 9	37.383 37. 7 47	1.00	85.19
	582	CB	SER C	76	14.101	44.448	37.402	1.00 1.00	85.19
20	583	OG	SER C	76	13.920	44.371	35.992	1.00	104.06 104.06
30	584	C	SER C	76	16.308	45.424	37.044	1.00	85.19
	585	0	SER C	76	16.560	46.020	35.998	1.00	85.19
	586 587	N CA	GLU C	77	17.140	44.553	37.612	1.00	76.77
	588	CA CB	GLU C	77	18.444	44.238	37.023	1.00	76.77
35	589	CG O	GLU C	77 77	19.263 19.643	43.355 44.039	37.962	1.00	228.57
	590	CD	GLU C	77	20.577	45.228	39.268 39.070	1.00	228.57
	591	OE1	GLU C	77	20.709	45.703	37.921	1.00 1.00	228.57
	592	OE2	GLU C	77	21.172	45.695	40.068	1.00	228.57 228.57
40	593	Ç	GLU C	77	18.178	43.498	35.728	1.00	76.77
40	594	0	GLU C	77	17.573	42.420	35.746	1.00	76.77
	595 596	N CD	PRO C	78	18.600	44.080	34.585	1.00	81.92
	597	CA	PRO C	78 78	19.176	45.434	34.463	1.00	75.82
	598	CB	PRO C	78	18.417 19.357	43.503 44.328	33.255	1.00	81.92
45	599	CG	PRO C	78	19.130	45.681	32.394 32.940	1.00 1.00	75.82
	600	С	PRO C	78	18.717	42.029	33.190	1.00	75.82 81.92
	601	0	PRO C	78	19.475	41.508	34.000	1.00	81.92
	602	N	VAL C	79	18.094	41.357	32.233	1.00	71.44
50	603 604	CA CB	VAL C	79	18.300	39.938	32.036	1.00	71.44
30	605	CG1	VAL C	79	17.121	39.139	32.538	1.00	74.89
	606	CG2	VAL C	79 79	17.199 17.131	37.717	32.029	1.00	74.89
	607	Č	VAL C	79	18.454	39.154 39.707	34.047	1.00	74.89
	608	Ō	VAL C	79	17.646	40.184	30.552 29.748	1.00	71.44
55	609	N	TYR C	80	19.502	38.989	30.179	1.00 1.00	71.44 69.00
	610	CA	TYR C	80	19.710	38.728	28.773	1.00	69.00
	611	CB	TYR C	80	21.184	38.7-7	28.406	1.00	132.22
	612 613	CG	TYR C	80	21.361	38.905	26.921	1.00	132.22
60	614	CD1 CE1	TYR C	80	20.962	40.075	26.284	1.00	132.22
00	615	CD2	TYR C	80 80	21.102	40.236	24.923	1.00	132.22
	616	CE2	TYR C	80	21.902 22.039	37.891 38.046	26.143	1.00	132.22
	617	CZ	TYR C	80	21.636	39.228	24.754 24.163	1.00	132.22
	618	ОН	TYR C	80	21.777	39.415	22.807	1.00 1.00	132.22 132.22
65	619	Ç	TYR C	80	19.150	37.401	28.300	1.00	69.00
	620	0	TYR C	80	19.295	36.380	28.939	1.00	69.00
	621	N CA	LEU C	81	18.534	37.423	27.141	1.00	61.97
	622 623	CA CB	LEU C	81	17.988	36.232	26.557	1.00	61.97
70	624	CB CG	LEU C	81 01	16.501	36.449	26.351	1.00	56.21
. •		•		81	15.878	35.304	25.589	1.00	56.21

	625	CD1	LEU C	81	.16.017	34.060	26.431	1.00	56.21
	626	CD2	LEU C	81	14.424	35.608	25.294	1.00	58.21
	627 628	CO	LEU C	81	18.700	36.019	25.213	1.00	61.97
5	629	Ň	GLU C	81 82	18.814 19.191	36.949 34.816	24.423	1.00	61.97
_	630	CA	GLU C	82	19.855	34.581	24.948 23.674	1.00	70.61
	631	CB	GLU C	82	21.326	34.242	23.882	1.00 1.00	70.61
	632	CG	GLU C	82	22.179	34.569	22.675	1.00	114.25 114.25
••	633	CD	GLU C	82	23.657	34.256	22.884	1.00	114.25
10	634	OE1	GLU C	82	24.149	34.456	24.020	1.00	114.25
	635	OE2	GLU C	82	24.331	33.827	21.913	1.00	114.25
	636	C	GLU C	82	19.172	33.457	22.896	1.00	70.61
	637 638	0 N	GLU C VAL C	82	18.913	32.381	23.440	1.00	70.61
15	639	CA CA	VAL C	83 83	18.886 18.225	33.706 32.717	21.622	1.00	70.46
	640	CB	VAL C	83	17.114	33.346	20.795 20.004	1.00	70.46
	641	CG1	VAL C	83	16.531	32.318	19.057	1.00 1.00	68.26 68.26
	642	CG2	VAL C	83	16.045	33.848	20.941	1.00	68.26
20	643	С	VAL C	83	19.156	32.014	19.825	1.00	70.46
20	644	0	VAL C	83	19.955	32.663	19.157	1.00	70.46
	645	N	PHE C	84	19.031	30.694	19.718	1.00	54.26
	646 647	CA CB	PHE C	84	19.913	29.944	18.845	1.00	54.26
	648	CG	PHE C PHE C	84 84	20.793 21.645	28.988	19.650	1.00	65.02
25	649	CD1	PHE C	84	21.045	29. 643 30.128	20.638	1.00	65.02
	650	CD2	PHE C	84	22.996	29. 7 67	21.788 20.426	1.00 1.00	65.02
	651	CE1	PHE C	84	21.897	30.746	22.733	1.00	65.02 65.02
	652	CE2	PHE C	84	23.811	30.384	21.359	1.00	65.02
20	653	CZ	PHE C	84	23.262	30.872	22.519	1.00	65.02
30	654	C	PHE C	84	19.247	29.092	17.790	1.00	54.26
	655 656	0	PHE C	84	18.045	28.781	17.861	1.00	54.26
	657	CA	SER C SER C	85 85	20.101	28.686	16.849	1.00	85.79
	658	CB	SER C	85	19.768 19.683	27.807 28.5 8 3	15.750 14.435	1.00	85.79
35	659	OG	SER C	85	19.375	27.719	13.355	1.00 1.00	134.11 134.11
	660	С	SER C	85	20.951	26.860	15.700	1.00	85.79
	661	0	SER C	85	22.063	27.274	15.360	1.00	85.79
	662	N	ASP C	86	20.731	25.607	16.083	1.00	52.64
40	663 664	CA CB	ASP C	86	21.798	24.604	16.049	1.00	52,64
70	665	CG	ASP C ASP C	86 86	22.912	24.984	17.015	1.00	115.87
	666	OD1	ASP C	86	24.265 24.448	24.581 23.384	16.504 16.194	1.00	115.87
	667	OD2	ASP C	86	25.144	25.459	16.411	1.00 1.00	115.87
	668	C	ASP C	86	21.199	23.235	16.420	1.00	115.87 52.64
45	669	0	ASP C	86	20.051	23.168	16.879	1.00	52.64
	670	N	TRP C	87	21.944	22.146	16.202	1.00	58.25
	671	CA	TRP C	87	21.424	20.809	16.522	1.00	58.25
	672 673	CB CG	TRP C TRP C	87	22.372	19.723	16.049	1.00	247.83
50	674	CD2	TRP C	87 87	22.083 22.700	19.354	14.675	1.00	247.83
-	675	CE2	TRP C	87	22.052	19.899 19.344	13.518 12.404	1.00 1.00	247.83
	676	CE3	TRP C	87	23.742	20.812	13.311	1.00	247.83 247.83
	677	CD1	TRP C	87	21.106	18.504	14.235	1.00	247.83
e e	678	NE1	TRP C	87	21.082	18.496	12.867	1.00	247.83
55	679	CZ2	TRP C	87	22.418	19.660	11.113	1.00	247.83
	680	CZ3	TRP C	87	24.098	21.132	12.023	1.00	247.83
	681 682	CH2 C	TRP C	87 97	23.444	∠0.552	10.944	1.00	247.83
	683	ŏ	TRP C	87 87	21.220 20.141	20.656 20.260	18.009	1.00	58.25
60	684	Ň	LEU C	88	22.264	20.985	18.463 18.760	1.00 1.00	58.25
	685	CA	LEU C	88	22.230	20.887	20.197	1.00	79.45 79.45
	686	CB	LEU C	88	23.225	19.845	20.659	1.00	57.97
	687	CG	LEU C	88	22.896	18.431	20.245	1.00	57.97
65	688	CD1	LEU C	88	23.876	17.490	20.880	1.00	57.97
UJ.	689 690	CD2	LEU C	88	21.495	18.114	20.693	1.00	57.97
	691	C	LEU C	88	22.558	22.194	20.870	1.00	79.45
	692	Ň	LEU C	88 89	23.432 21.872	22.940 22.451	20.419	1.00	79.45
	693	CA	LEU C	89	22.097	22.451 23.669	21.976 22.732	1.00	57.52 57.50
70	694	СВ	LEU C	89	20.919	24.616	22.578	1.00 1.00	57.52 59.32
									30.32

	695	CG	LEU C	89	- 21.105	25.884	23.373	1.00	59.32
	696 697	CD1 CD2	LEU C	89	22.513	26.439	23.134	1.00	59.32
	698	C .	LEU C	89 89	20.081 22.246	26.861 23.316	22.941	1.00	59.32
5	699	ŏ	LEU C	89	21.432	22.577	24.184 24.697	1.00 1.00	57.52
	700	N	LEU C	90	23.287	23.815	24.846	1.00	57.52 64.90
	701	CA	LEU C	90	23.472	23.521	26.267	1.00	64.90
	702 703	CB CG	LEU C	90	24.948	23.512	26.638	1.00	46.55
10	703	CD1	LEU C	90 90	25.227 24.701	23.312 21.955	28.119	1.00	46.55
••	705	CD2	LEU C	90	26.712	23.409	28.491 28.423	1.00 1.00	46.55
	706	C	LEU C	90	22.781	24.591	27.083	1.00	46.55 64.90
	707	0	LEU C	90	23.167	25.754	27.032	1.00	64.90
15	708	N	GLN C	91	21.769	24.208	27.852	1.00	56.08
13	709 710	CA CB	GLN C GLN C	91	21.052	25.187	28.650	1.00	56.08
	711	CG	GLN C	91 91	19.573 19.115	24.944 25.036	28.517 27.094	1.00	49.57
	712	CD	GLN C	91	17.606	25.013	27.094 26.979	1.00 1.00	49.57
•	713	OE1	GLN C	91	16.947	23.977	27.245	1.00	49.57 49.57
20	714	NE2	GLN C	91	17.030	26.167	26.601	1.00	49.57
	715	C	GLN C	91	21.440	25.146	30.103	1.00	56.08
	716 717	O N	GLN C ALA C	91 92	21.697	24.066	30.638	1.00	56.08
	718	· CA	ALA C	92	21.494 21.852	26.309 26.335	30.752 32.166	1.00	47.15
25	719	CB	ALA C	92	23.160	26.962	32.345	1.00 1.00	47.15
	720	С	ALA C	92	20.828	27.102	32.955	1.00	42.48 47.15
	721	0	ALA C	92	20.300	28.102	32.474	1.00	47.15
	722	N	SER C	93	20.510	26.620	34.151	1.00	67.10
30	723 724	CA CB	SER C SER C	93	19.541	27.289	35.013	1.00	67.10
50	725	OG	SER C	93 93	19.475 20.758	26.625 26,434	36.392	1.00	100.79
	726	č	SER C	93	20.758	28.705	36.965 35.137	1.00 1.00	100.79 67.10
	727	0	SER C	93	19.395	29.632	34.692	1.00	67.10
25	728	N	ALA C	94	21.220	28.868	35.704	1.00	57.34
35	729	CA	ALA C	94	21.818	30.179	35.875	1.00	57.34
	730 731	CB C	ALA C ALA C	94	21.716	30.609	37.326	1.00	92.07
	732	ŏ	ALA C	94 94	23.279 23.912	30.072 29.048	35.462	1.00	57.34
	733	Ň	GLU C	95	23.825	31.123	35.694 34.860	1.00 1.00	57.34 69.09
40	734	CA	GLU C	95	25.212	31.088	34.419	1.00	69.09
	735	CB	GLU C	95	25.403	31.994	33.214	1.00	142.79
	736	CG	GLU C	95	24.526	31.618	32.048	1.00	142.79
	737 738	CD OE1	GLU C	95 95	24.954 24.268	32.288	30.759	1.00	142.79
45	739	OE2	GLU C	95	25.976	32.084 33.013	29.733 30.767	1.00 1.00	142.79 142.79
	740	c c	GLU C	95	26.232	31.459	35.494	1.00	69.09
	741	0	GLU C	95	27.435	31.238	35.316	1.00	69.09
	742	N	VAL C	96	25.765	32.041	36.598	1.00	86.41
50	743 744	CA CB	VAL C	96	26.640	32.419	37.713	1.00	86.41
50	745	CG1	VAL C VAL C	96 96	26.922 28.119	33.903	37.702	1.00	74.25
	746	CG2	VAL C	96	27.176	34.207 34.357	38.587 36.277	1.00 1.00	74.25
	747	C	VAL C	96	25.910	32.052	38.990	1.00	74.25 86.41
	748	0	VAL. C	96	24.733	32.348	39.135	1.00	86.41
55	749	N.	VAL C	97	26.610	31.434	39.931	1.00	73.13
	750 751	CA	VAL C	97	25.953	30.955	41.142	1.00	73.13
	751 752	CB CG1	VAL C VAL C	97 97	25.697 24.767	29.456 28.999	41.001	1.00	48.19
	753	CG2	VAL C	97	25.176	29.146	42.037 39.634	1.00 1.00	48.19
60	754	C	VAL C	97	26.715	31.125	42.448	1.00	48.19 73.13
	755	0	VAL C	97	27.924	30.893	42.513	1.00	73.13
	756	N	MET C	98	25.999	31.490	43.503	1.00	70.97
	757 750	CA	MET C	98	26.612	31.622	44.828	1.00	70.97
65	758 759	CB CG	MET C MET C	98 98	25.638 25.295	32.331	45.763	1.00	151.84
	760	SD	MET C	98	25.295 26.581	33.728 34.857	45.318 45.790	1.00	151.84
	761	CE	MET C	98	26.247	34.962	45.790 47.553	1.00 1.00	151.84 151.84
	762	С	MET C	98	26.930	30.228	45.380	1.00	70.97
70	763	0	MET C	98	26.094	29.335	45.348	1.00	70.97
70	764	N	GLU C	99	28.130	30.037	45.923	1.00	61.59

	765	CA	GLU C	99	28.508	28.740	48.475	1.00	••
	768	СВ	GLU C	99	29.762	28.874	47.339	1.00 1.00	61.59 200.85
	767	CG	GLU C	89	30.525	27.574	47.520	1.00	200.85
_	768 .	CD	GLU C	. 88	31.561	27.657	48.623	1.00	200.85
5	769	OE1	GLU C	99	32.197	28.724	48.761	1.00	200.85
	770 771	OE2	GLU C	99	31.746	26.651	49.342	1.00	200.85
	772	C	GLU C	99 99	27.354	28.221	47.325	1.00	61.59
	773	Ň	GLY C	100	26.851 26.901	28.934 27.000	48.184	1.00	61.59
10	774	CA	GLY C	100	25.819	26.456	47.076 47.876	1.00 1.00	69.94
	775	С	GLY C	100	24.468	26.355	47.191	1.00	69.94 69.94
	776	0	GLY C	100	23.600	25.591	47.657	1.00	69.94
	777	N	GLN C	101	24.266	27.111	46.105	1.00	57.42
15	778	CA	GLN C	101	22.990	27.083	45.370	1.00	57.42
13	779 730	CB CG	GLN C	101	22.778	28.399	44.634	1.00	124.38
	730 781	CD	GLN C	101 101	22.627 21.628	29.570 29.295	45.551	1.00	124.38
	782	OE1	GLN C	101	21.911	28.587	46.641 47.605	1.00 1.00	124.38
	783	NE2	GLN C	101	20.438	29.839	46.485	1.00	124.38 124.38
20	784	C	GLN C	101	22.854	25.918	44.369	1.00	57.42
	785	0	GLN C	101	23.834	25 £_3	44.031	1.00	57.42
	786 787	N CD	PRO C	102	21.627	25.663	43.893	1.00	52.71
	788	CA.	PRO C PRO C	102 102	20.356	26.358	44.165	1.00	80.58
25	789	CB	PRO C	102	21.438 19.957	24.573 24.318	42.942	1.00	52.71
	790	CG	PRO C	102	19.422	25.709	43.044 43.171	1.00 1.00	80.58
	791	С	PRO C	102	21.870	25.005	41.531	1.00	80.58 52.71
	782	· O	PRO C	102	21.853	26.203	41.189	1.00	52.71
20	793	N	LEU C	103	22.242	24.033	40.705	1.00	64.68
30	794 795	CA	LEU C	103	22.661	24.323	39.343	1.00	64.68
	796	CB CG	LEU C	103	24.172	24.347	39.273	1.00	81.00
	797	CD1	LEU C	103 103	24.605 24.136	24.608 25.987	37.838 37.435	1.00	81.00
	798	CD2	LEU C	103	26.113	24.486	37.718	1.00 1.00	81.00 81.00
35	799	C	LEU C	103	22.147	23.244	38.403	1.00	64.68
	800	0	LEU C	103	22.418	22.063	38.642	1.00	64.68
	801	N	PHE C	104	21.409	23.616	37.355	1.00	64.85
	802 803	CA CB	PHE C	104	20.923	22.599	36.423	1.00	64.85
40	804	CG	PHE C	104 104	19.392 18.787	22.530 22.248	36.418	1.00	111.94
	805	CD1	PHE C	104	18.694	23.250	37.758 38.710	1.00 1.00	111.94
	806	CD2	PHE C	104	18.300	20.980	38.068	1.00	111.94 111.94
	807	CE1	PHE C	104	18.128	23.000	39.962	1.00	111.94
45	808	CE2	PHE C	104	17.731	20.717	39.320	1.00	111.94
43	809 810	CZ C	PHE C	104	17.844	21.732	40.268	1.00	111.94
	811	. 0	PHE C	104 104	21.410 21.254	22.829	34.993	1.00	64.85
	812	Ň	LEU C	105	22.009	23.915 21.817	34.462 34.371	1.00	64.85
	813	CA	LEU C	105	22.469	21.933	32.983	1.00 1.00	49.42 49.42
50	814	CB	LEU C	105	23.928	21.502	32.848	1.00	35.01
	815	CG	LEU C	105	24.870	22.289	33.757	1.00	35.01
	816	CD1	LEU C	105	26.346	21.971	33.451	1.00	35.01
	817 818	CD2 C	LEU C	105	24.579	23.735	33.535	1.00	35.01
55	819	ŏ	LEU C	105 105	21.603 21.225	21.000 19.954	32.181	1.00	49.42
	820	N	ARG C	106	21.290	21.353	32.679 30.946	1.00	49.42
	821	CA	ARG C	106	20.438	20.487	30.155	1.00 1.00	67.77 67.77
	822	CB	AHG C	108	19.027	21.043	30.194	1.00	104.09
60	823	ca	ARG C	106	18.058	20.302	29.334	1.00	104.09
w	824 825	CD	ARG C	106	16.745	21.071	29.217	1.00	104.09
	826	NE CZ	ARG C ARG C	106 106	15.814	20.401	28.316	1.00	104.09
	827	NH1	ARG C	106	14.812 14.616	21.002 22.292	27.694 27.870	1.00	104.09
	828	NH2	ARG C	106	14.023	20.314	27.879 26.879	1.00 1.00	104.09 104.09
65	829	C	ARG C	106	20.911	20.391	28.710	1.00	67.77
	830	Ö	ARG C	106	21.063	21.431	28.053	1.00	67.77
	831	N	CYS C	107	21.160	19.179	28.205	1.00	64.22
	832 833	CA C	CYS C	107	21.599	19.074	26.819	1.00	64.22
70	834	ŏ	CYS C	107 107	20.320 19.579	19.044	26.063	1.00	64.22
. •		-	0.0	.07	10.018	18.067	26.143	1.00	64.22

	š	CB	CYS C	107	.22.396	17.808	26.547	1.00	74.81
	J6	SG	CYS C	107	23.369	17.892	24.999	1.00	74.81
	37 138	N _.	HIS C	108	20.054	20.132	25.351	1.00	62.02
	.139	. CA	HIS C	108	18.815	20.288	24.593	1.00	62.02
	140	CB CG	HIS C HIS C	108 108	18.257	21.669	24.859	1.00	73.41
	.141	CD2	HIS C	108	16.893 16.409	21.884 22.839	24.302 23.479	1.00	73.41
	842	ND1	HIS C	108	15.821	21.093	24.848	1.00	73.41
٠.	843	CE1	HIS C	108	14.731	21.558	24.067	1.00 1.00	73.41
	844	NE2	HIS C	108	15.061	22.618	23.353	1.00	73.41 73.41
	845	Ç	HIS C	108	18.925	20.085	23.089	1.00	62.02
	846	0	HIS C	108	19.750	20.724	22.412	1.00	62.02
	847 848	N CA	GLY C	109	18.066	19.207	22.578	1.00	82.12
15	849	c	GLY C	109 109	18.075	18.907	21.161	1.00	82.12
	850	ŏ	GLY C	109	17.196 16.281	19.859 20.439	20.396 20.963	1.00	82.12
	851	N	TRP C	110	17.473	20.020	19.107	1.00	82.12
	852	CA	TRP C	110	16.691	20.916	18.282	1.00 1.00	66.53
20	853	CB	TRP C	110	17.327	21.057	16.911	1.00	· 66.53 113.55
20	854	CG	TRP C	110	16.487	21.825	15.969	1.00	113.55
	855 856	CD2 CE2	TRP C	110	16.565	23.226	15.701	1.00	113.55
	857	CE3	TRP C	110	15.552	23.532	14.769	1.00	113.55
	858	CD1	TRP C	110 110	17.401	24.260	16.157	1.00	113.55
25	859	NE1	TRP C	110	15.460 14.892	21.348 22.364	15.216	1.00	113.55
	860	CZ2	TRP C	110	15.345	24.831	14.490 14.280	1.00	113.55
	861	CZ3	TRP C	110	17.193	25.561	15.668	1.00 1.00	113.55
	862	CH2	TRP C	110	16.171	25.829	14.742	1.00	113.55
30	863 864	C	TRP C	110	15.284	20.383	18.160	1.00	113.55 66.53
50	865	0 N	TRP C	116	15.060	19.188	18.276	1.00	66.53
	868	CA	ARG C ARG C	111	14.334	21.285	17.951	1.00	82.69
	867	CB	ARG C	111 111	12.928 12.677	20.924	17.807	1.00	82.69
	888	CG	ARG C	111	12.367	20.368	16.432	1.00	249.07
35	869	CD	ARG C	111	11.908	21.439 20.831	15.493 14.270	1.00	249.07
	870	NE	ARG C	111	10.767	21.587	13.769	1.00 1.00	249.07
	871	cz	ARG C	111	9.568	21.660	14.334	1.00	249.07 249.07
	872 873	NH1 NH2	ARG C	111	9.309	20.994	15.438	1.00	249.07
40	874	rinz C	ARG C ARG C	111	8.601	22.346	13.736	1.00	249.07
	875	ŏ	ARG C	111 111	12.433 11.471	19.928	18.828	1.00	82.69
	876	N	ASN C	112	13.119	19.213	18.595	1.00	82.69
	877	-CA	ASN C	112	12.756	19.872 18.976	19.953 21.027	1.00	79.91
45	878	CB	ASN C	112	11.354	19.288.	21.540	1.00 1.00	79.91
45	879	CG	ASN C	112	11.152	18.815	22.957	1.00	134.30 134.30
	880 881	OD1 ND2	ASN C	112	11.850	17.902	23.427	1.00	134.30
	882	C	ASN C ASN C	112	10.194	19.424	23.653	1.00	134.30
	883	ŏ	ASN C	112 112	12.833	17.513	20.651	1.00	79.91
50	884	Ň	TRP C	113	12.172 13.637	16.683	21.270	1.00	79.91
	885	CA	TRP C	113	13.771	17.180 15.780	19.650	1.00	91.68
	888	CB	TRP C	113	14.648	15.601	19.287 18.062	1.00	91.68
	887	CG	TRP C	113	13.958	15.923	16.805	1.00 1.00	105.58
55	889	CD2 CE2	TRP C	113	14.528	16.557	15.662	1.00	105.58 105.58
33	890	CE2 CE3	TRP C	113	13.524	16.609	14.670	1.00	105.58
	891	CD1	TRP C	113 113	15.803	17.083	15.373	1.0	105.58
	892	NE1	TRP C	110	12.660 12.393	15.629	16.478	1.00	105.58
	893	CZ2	TRP C	113	13.750	16.038 17.164	15.194 13.413	1.00	105.58
60	894	CZ3	TRP C	113	16.030	17.637	14.119	1.00 1.00	105.58
	895	CH2	TRP C	113	15.005	17.676	13.155	1.00	105.58
	896	C	TRP C	113	14.393	15.003	20.425	1.00	105.58 91.68
	. 897 898	0 N	TRP C	113	14.528	15.502	21.543	1.00	91.68
65	899	ČA	ASP C ASP C	114	14.780	13.770	20.133	1.00	96.80
	900	ČB	ASP C	114 114	15.398 14.675	12.926	21.133	1.00	96.80
	901	CG	ASP C	114	13.402	11.576 11.645	21.213	1.00	249.33
	902	OD1	ASP C	114	13.493	12.001	22.044 23.239	1.00	249.33
70	903	ODS	ASP C	114	12.314	11.344	21.507	1.00	249.33
70	904	С	ASP C	114	16.886	12.727	20.813	1.00 1.00	249.33
									96.80

	905	0	ASP C	444	47.057	40 504	40.000		
	906	N	ASP C VAL C	114 115	. 17.257 17.678	12.561 12.771	19.652	1.00	96.80
	907	ĞA	VAL C	115	19.112	12.771	21.860 21.728	1.00	71.72
	908	CB	VAL C	115	19.875	13.783	22.274	1.00 1.00	71.72
5	909	CG1	VAL C	115	21.344	13.665	21.884	1.00	77.93 77.93
	910	CG2	VAL C	115	19.257	15.061	21.751	1.00	77.93
	911	С	VAL C	115	19.535	11,382	22.516	1.00	71.72
	912	0	VAL C	115	18.999	11,111	23.589	1.00	71.72
10	913	N	TYR C	116	20.502	10.653	21.979	1.00	67.55
10	914 915	CA CB	TYR C	116	20.999	9.454	22.644	1.00	67.55
	916	CG	TYR C TYR C	116	20.610	8.219	21.826	1.00	100.42
	917	CD1	TYR C	116 116	19.121 18.431	8.010 8.465	21.689	1.00	100.42
	918	CE1	TYR C	116	17.049	8.284	20.572 20.454	1.00 1.00	100.42
15	919	CD2	TYR C	116	18.403	7.371	22.690	1.00	100.42 100.42
	920	CE2	TYR C	116	17.028	7.185	22.590	1.00	100.42
	921	CZ	TYR C	116	16.352	7.644	21.468	1.00	100.42
	922	ÓН	TYR C	116	14.991	7.468	21.357	1.00	100.42
20	923	C	TYR C	116	22.514	9.501	22.853	1.00	67.55
20	924	0	TYR C	116	23.187	10.404	22.351	1.00	67.55
	925 926	N CA	LYS C LYS C	117	23.040	8.518	23.578	1.00	124.33
	927	CB	LYS C	117 117	24.466 25.233	8.443 7.946	23.848	1.00	124.33
	928	CG	LYS C	117	25.233 25.319	7.946 6.439	22.617 22.465	1.00	168.92
25	929	CD	LYS C	117	26.431	6.073	21.494	1.00 1.00	168.92
	930	CE	LYS C	117	27.782	6.589	21.988	1.00	168.92 168.92
	931	NZ	LYS C	117	28.904	6.284	21.056	1.00	168.92
	932	Ç	LYS C	117	24.974	9.822	24.229	1.00	124.33
30	933	0	LYS C	117	25.904	10.347	23.608	1.00	124.33
30	934	N	VAL C	118	24.361	10.406	25.253	1.00	96.88
	935 936	CA CB	VAL C VAL C	118	24.752	11.731	25.714	1.00	96.88
	937	CG1	VAL C	118 118	23.572 24.036	12.432 13.463	26.338	1.00	47.91
	938	CG2	VAL C	118	22.786	13.114	27.307 25.264	1.00 1.00	47.91
35	939	C	VAL C	118	25.914	11.799	26.692	1.00	47.91 96.88
	940	0	VAL C	118	25.980	11.030	27.648	1.00	96.88
	941	Ņ	ILE C	119	26.815	12.746	26.455	1.00	44.35
	942	CA	ILE C	119	27.968	12.917	27.316	1.00	44.35
40	943 944	CB	ILE C	119	29.214	12.377	26.650	1.00	99.63
40	944	CG2 CG1	ILE C	119 119	30.395	12.468	27.585	1.00	99.63
	946	CD1	ILE C	119	28.973 30.044	10.939 10.421	26.239 25.239	1.00	99.63
	947	Č.	ILE C	119	28.227	14.396	25.309 27.618	1.00 1.00	99.63
	948	0	ILE C	119	28.466	15.166	26.683	1.00	44.35 44.35
45	949	N	TYR C	120	28.193	14.816	28.889	1.00	48.39
	950	CA	TYR C	120	28.478	16.224	29.185	1.00	48.39
	951	CB	TYR C	120	27.803	16.687	30.458	1.00	42.29
	952 953	CG CD1	TYR C	120	26.322	16.785	30.363	1.00	42.29
50	954	CE1	TYR C	120	25.537	15.697	30.581	1.00	42.29
50	955	CD2	TYR C	120 120	24.185 25.710	15.775 17.982	30.485 30.035	1.00	42.29
	956	CE2	TYR C	120	24.340	18.088	29.924	1.00 1.00	42.29
	957	CZ	TYR C	120	23.584	16.968	30.155	1.00	42,29
	958	OH	TYR C	120	22.206	17.007	30.061	1.00	42.29 42.29
55	959	Ç	TYR C	120	29.962	16.358	29.412	1.00	48.39
	960	0	TYR C	120	30.602	15.447	29.935	1.00	48.39
	961	N	TYR C	121	30.518	17.498	29.053	1.00	53.29
	962 963	CA CB	TYR C	121	31.942	17.700	29.246	1.00	53.29
60	964	CG	TYR C TYR C	121	32.664 32.747	17.828	27.887	1.00	75.15
-	965	CD1	TYR C	121 121	31.598	16.569 15.071	27.044	1.00	75.15
	966	CE1	TYR C	121	31.669	15.971 14.849	26.525 25.717	1.00 1.00	75.15 75.15
	967	CD2	TYR C	121	33.976	16.002	26.731	1.00	75.15 75.15
15	968	CE2	TYR C	121	34.055	14.881	25.921	1.00	75.15 75.15
65	969	CZ	TYR C	121	32.895	14.315	25.421	1.00	75.15
	970	он	TYR C	121	32.960	13.214	24.613	1.00	75.15
	971 972	C	TYR C	121	32.219	18.966	30.056	1.00	53.29
	973	0 N	TYR C LYS C	121	31.547	19.984	29.872	1.00	53.29
70	974	CA	LYS C	122 122	33.199 33.580	18.908	30.954	1.00	72.38
		3 A		122	JJ.J0U	20.077	31.725	1.00	72.38

	975	CB	LYS C	122	- 33.217	19.930	33.197	1.00	00.00
	976	CG	LYS C	122	33.582	21.162	34.003	1.00	98.98 98.98
	977	CD	LYS C	122	33.532	20.901	35.481	1.00	98.98
_	978 .	CE	LYS C	122	34.071	22.074	36.260	1.00	98.98
5	979	NZ	LYS C	122	34.151	21.706	37.694	1.00	98.98
	980	C	LYS C	122	35.080	20.238	31.595	1.00	72.38
	981 982	O N	LYS C ASP C	122	35.836	19.379	32.017	1.00	72.38
	983	CA	ASP C	123 123	35.507 36.918	21.342 21.628	31.001	1.00	92.01
10	984	CB	ASP C	123	37.606	21.819	30.809 32.161	1.00	92.01
	985	CG	ASP C	123	37.288	23.167	32.785	1.00 1.00	107.76
	986	OD1	ASP C	123	37.362	24.186	32.052	1.00	107.76 107.76
	987	OD2	ASP C	123	36.979	23.215	34.000	1.00	107.76
	988	С	ASP C	123	37.613	20.553	29.996	1.00	92.01
15	989	0	ASP C	123	38.719	20.144	30.322	1.00	92.01
	990	N	GLY C	124	36.956	20.110	28.929	1.00	87.40
	991 992	CA	GLY C	124	37.516	19.094	28.054	1.00	87.40
	993	C O	GLY C	124 124	37.465	17.665	28.570	1.00	87.40
20	994	Ň	GLU C	125	37.795 37.047	16.741 17.474	27.826 29.821	1.00	87.40
	995	CA	GLU C	125	36.991	16.139	30.427	1.00 1.00	63.88
	996	СВ	GLU C	125	37.331	16.197	31.931	1.00	63.88 184.13
	997	CG	GLU C	125	38.775	16.547	32.294	1.00	184.13
0.5	998	CD	GLU C	125	39.723	15.367	32.176	1.00	184.13
25	999	OE1	GLU C	125	39.524	14.369	32.903	1.00	184.13
	1000	OE2	GLU C	125	40.665	15.445	31.359	1.00	184.13
	1001 1002	C O	GLU C	125	35.626	15.490	30.284	1.00	63.88
	1002	Ň	ALA C	125 126	34.611 35.587	16.164	30.370	1.00	63.88
30	1004	CA	ALA C	126	34.302	14.182 13.501	30.067 29.985	1.00	91.37
-	1005	CB	ALA C	126	34.516	12.040	29.654	1.00 1.00	91.37 171.72
	1006	C	ALA C	126	33.727	13.657	31.399	1.00	91.37
	1007	0	ALA C	126	34.492	13.626	32.369	1.00	91.37
25	1008	N	LEU C	127	32.410	13.835	31.533	1.00	55.93
35	1009	CA	LEU C	127	31.815	14.011	32.861	1.00	55.93
	1010 1011	CB CG	LEU C	127	31.291	15.421	33.033	1.00	79.78
	1012	CD1	LEU C	127 127	31.277 32.708	15. 727 15.528	34.519	1.00	79.78
	1013	CD2	LEU C	127	30.796	17.133	35.062 34.754	1.00 1.00	79.78
40	1014	C	LEU C	127	30.722	13.050	33.267	1.00	79.78 55.93
	1015	0	LEU C	127	30.851	12.396	34.292	1.00	55.93
	1016	N	LYS C	128	29.633	12.998	32.501	1.00	71.66
	1017	CA ·	LYS C	128	28.530	12.063	32.771	1.00	71.66
45	1018 1019	CB CG	LYS C	128	27.354	12,774	33.419	1.00	111.82
73	1020	CD	LYS C	128 128	27.672 27.814	13.421	34.740	1.00	111.82
	1021	CE	LYS C	128	27.814	12,412 13,133	35.853 37.204	1.00	111.82
	1022	NZ	LYS C	128	28.021	12.205	38.387	1.00 1.00	111.82 111.82
	1023	С	LYS C	128	28.096	11.462	31.430	1.00	71.66
50	1024	0	LYS C	128	28.281	12.090	30.386	1.00	71.66
	1025	N	TYR C	129	27.537	10.252	31.447	1.00	51.68
	1026	CA	TYR C	129	27.110	9.616	30.208	1.00	51.68
	1027	CB	TYR C	129	28.197	8.680	29.692	1.00	75.51
55	1028 1029	CG CD1	TYR C	129	27.655	7.647	28.732	1.00	75.51
33	1030	CE1	TYR C	129 129	27.412 26.846	7.957 7.041	27.399	1.00	75.51
	1031	CD2	TYR C	129	27.316	6.383	26.529 29.173	1.00	75.51
	1032	CE2	TYR C	129	26.739	5.454	28.309	1.00 1.00	75.51 75.51
<i>c</i> 0	1033	CZ	TYR C	129	26.510	5.789	26,992	1.00	75.51
60	1034	ÓН	TYR C	129	25.950	4.855	26.144	1.00	75.51
	1035	C	TYR C	129	25.817	8.822	30.371	1.00	51.68
	1036 1037	O	TYR C	129	25.656	8.097	31.360	1.00	51.68
	1037	N CA	TRP C	130	24.912	8.945	29.390	1.00	122.00
65	1039	CB	TRP C	130 130	23.641 22.531	8. 22 6 9.082	29.404	1.00	122.00
	1040	ČĠ	TRP C	130	22.854	9.082 9.740	29.995 31.299	1.00	131.84
	1041	CD2	TRP C	130	22.370	9.360	32.590	1.00 1.00	131.84 131.84
	1042	CE2	TRP C	130	22.886	10.292	33.518	1.00	131.84 131.84
70	1043	CE3	TRP C	130	21.557	8.317	33.053	1.00	131.84
70	1044	CD1	TRP C	130	23.613	10.850	31.489	1.00	131.84

	1045 1046	NE1 CZ2	TRP C	130 130	23.636 22.613	11.194 10.216	32.819	1.00	131.84
	1047	CZ3	TRP C	130	21.283	8.239	34.887 34.422	1.00	131.84
	1048	CH2	TRP C	130	21.809	9.190	35,319	1.00 1.00	131.84
5	1049	С	TRP C	130	23.199	7.805	28.010	1.00	131.84 122.00
	1050	0	TRP C	130	23.720	8.292	27.015	1.00	122.00
	1051	N	TYR C	131	22.229	6.898	27.944	1.00	94.11
	1052	CA	TYR C	131	21.710	6.443	26.663	1.00	94.11
10	1053 1054	CB CG	TYR C	131	21.108	5.048	26.756	1.00	199.39
10	1055	CD1	TYR C	131 131	20.805 21.836	4.505	25.386	1.00	199.39
	1056	CE1	TYR C	131	21.583	4.074 3.681	24.552 23.247	1.00	199.39
	1057	CD2	TYR C	131	19.503	4.522	24.879	1.00 1.00	199.39
	1058	CE2	TYR C	131	19.236	4.132	23.570	1.00	199.39 199.39
15	1059	CZ	TYR C	131	20.283	3.716	22.761	1.00	199.39
	1060	OH	TYR C	131	20.033	3.369	21.456	1.00	199.39
	1061	C	TYR C	131	20.629	7.440	26.306	1.00	94.11
	1062	0	TYR C	131	20.894	8.379	25.554	1.00	94.11
20	1063	N	GLU C	132	19.411	7.221	26.817	1.00	108.28
20	1064 1065	CA CB	GLU C	132	18.318	8.171	26.599	1.00	108.28
	1066	CG	GLU C	132 132	16.986	7.670	27.185	1.00	249.42
	1067	CD	GLU C	132	16.250 14.874	6.597 7.058	26.375 25.901	1.00	249.42
	1068	OE1	GLU C	132	14.343	8.036	26.469	1.00 1.00	249.42
25	1069	OE2	GLU C	132	14.320	6.434	24.968	1.00	249.42 249.42
	1070	С	GLU C	132	18.899	9.243	27.491	1.00	108.28
	1071	0	GLU C	132	19.243	8.953	28.636	1.00	108.28
	1072	, N	ASN C	133	19.029	10.468	26.989	1.00	132.29
20	1073	CA	ASN C	133	19.665	11.502	27.790	1.00	132.29
30	1074	CB	ASN C	133	19.946	12.758	26.960	1.00	123.07
	1075 1076	CG OD1	ASN C	133	18.786	13.702	26.928	1.00	123.07
	1077	ND2	ASN C ASN C	133	17.659	13.297	26.651	1.00	123.07
	1078	C	ASN C	133 133	19.047 18.983	14.979	27.200	1.00	123.07
35	1079	ŏ	ASN C	133	17.884	11.879 11.434	29.090 29.412	1.00 1.00	132.29
	1080	N	HIS C	134	19.877	12.730	29.824	1.00	132.29 77.87
	1081	CA	HIS C	134	19.271	13.173	31.140	1.00	77.87 77.87
	1082	C8	HIS C	134	20.089	12.388	32.162	1.00	247.23
40	1083	CG	HIS C	134	19.688	12.628	33.579	1.00	247.23
40	1084	CD2	HIS C	134	20.384	13.171	34.619	1.00	247.23
	1085 1086	ND1 CE1	HIS C	134	18.451	12.270	34.071	1.00	247.23
	1087	NE2	HIS C	134	18.385	12.581	35.352	1.00	247.23
	1088	C	HIS C	134 134	19.532 19.573	13.127 14.664	35.710	1.00	247.23
45	1089	ŏ	HIS C	134	19.843	15.338	31.255 30.252	1.00 1.00	77.87
	1090	Ň	ASN C	135	19.539	15.167	32.484	1.00	77.87 77.12
	1091	CA	ASN C	135	19.779	16.576	32.747	1.00	77.12 77.12
	1092	CB	ASN C	135	18.442	17.308	32.868	1.00	227.67
50	1093	CG	ASN C	135	17.690	17.335	31.558	1.00	227.67
50	1094	OD1	ASN C	135	18.287	17.624	30.520	1.00	227.67
	1095 1096	ND2	ASN C	135	16.390	17.049	31.585	1.00	227.67
	1097	C O	ASN C ASN C	135	20.595 20.049	16.748	34.004	1.00	77.12
	1098	Ň	ILE C	135 136	21.914	16.927 16.671	35.075 33.862	1.00	77.12
55	1099	CA	ILE C	136	22.855	16.810	34.974	1.00 1.00	56.71
	1100	CB	ILE C	136	24.267	17.147	34.439	1.00	56.71 111.08
	1101	CG2	ILE C	136	24.215	18.298	33.468	1.00	111.08
	1102	CG1	ILE C	136	25.189	17.479	35.590	1.00	111.08
60	1103	CD1	ILE C	136	26.605	17.684	35.143	1.00	111.08
00	1104	C	ILE C	136	22.387	17.870	35.956	1.00	56.71
	1105 1106	0 N	ILE C SER C	136	22.276	19.044	35.623	1.00	58.71
	1107	CA	SER C	137	22.090	17.429	37.172	1.00	99.75
	1108	CB	SER C	137 137	21.594 20.218	18.308	38.225	1.00	99.75
65	1109	õõ	SER C	137	19.833	17.820 18.438	38.673 39.884	1.00 1.00	125.93 125.93
	1110	Č	SER C	137	22.517	18.411	39.437	1.00	125.93 99.75
	1111	O	SER C	137	23.195	17.457	39.807	1.00	99.75
	1112	N	ILE C	138	22.530	19.580	40.062	1.00	72.38
70	1113	CA	ILE C	138	23.366	19.816	41.235	1.00	72.38
70	1114	СВ	ILE C	138	24.560	20.663	40.881	1.00	52.39

	1115	CG2	ILE C	138	·25.241	21,106	42.161	1.00	52.39
	1116	CG1	ILE C	138	25.503	19.881	39.961	1.00	52.39
	1117	CD1	ILE C	138	26.574	20.747	39.311	1.00	52.39
5	1118	Ç	ILE C	138	22.609	20.556	42.335	1.00	72.38
5	1119 1120	O N	ILE C	138 139	22.109	21.667	42 .112	1.00	72.38
	1121	CA	THR C	139	22.535 21.823	19.955 20.568	43.519	1.00	119.29
	1122	CB	THR C	139	21.466	19.521	44.634 45.682	1,00 1.00	119.29
	1123	OG1	THR C	139	22.642	8.774	46.024	1.00	137.72
10	1124	CG2	THR C	139	20.404	18.578	45.139	1.00	137.72 137.72
	1125	С	THR C	139	22.679	21.655	45.275	1.00	119.29
	1126	0	THR C	139	22.449	22.849	45.063	1.00	119.29
	1127	N	ASN C	140	23.661	21.232	46.066	1.00	83.41
15	1128	CA	ASN C	140	24.585	22.147	46.730	1.00	83.41
13	1129 1130	CB CG	ASN C ASN C	140	25.065	21.554	48.052	1.00	209.19
	1131	OD1	ASN C	140 140	26.123 27.087	22.402 22.824	48.714	1.00	209.19
	1132	ND2	ASN C	140	25.950	22.624 22.645	48.073 50.006	1.00	209.19
	1133	C	ASN C	140	25.758	22.277	45.780	1.00 1.00	209.19 83.41
20	1134	Ō	ASN C	140	26.403	21.277	45.455	1.00	83.41
	1135	N	ALA C	141	26.037	23.503	45.343	1.00	87.00
	1136	CA	ALA C	141	27.121	23.741	44.394	1.00	87.00
	1137	СВ	ALA C	141	26.704	24.753	43.381	1.00	58.59
25	1138	Ç	ALA C	141	28.440	24.162	44.994	1.00	87.00
25	1139	0	ALA C	141	28.527	25.112	45.753	1.00	87.00
	1140	N	THR C	142	29.485	23.450	44.617	1.00	69.33
	1141 1142	CA CB	THR C	142	30.822	23.733	45.106	1.00	69.33
	1143	OG1	THR C	142 142	31.688 31.001	22.461 21.383	45.035 45.687	1.00	195.23
30	1144	CG2	THR C	142	33.012	21.363 22.679	45.722	1.00 1.00	195.23
	1145	Č	THR C	142	31.388	24.815	44,202	1.00	195.23 69.33
	1146	Ö	THR C	142	30.753	25.185	43.219	1.00	69.33
	1147	N	VAL C	143	32.561	25.341	44.531	1.00	71.38
25	1148	CA	VAL C	143	33.154	26.387	43.699	1.00	71.38
35	1149	CB	VAL C	143	34.082	27.349	44.511	1.00	62.36
	1150	CG1	VAL C	143	35.270	26.572	45.059	1.00	62.36
	1151 1152	CG2 C	VAL C	143	34.571	28.506	43.623	1.00	62.36
	1153	ŏ	VAL C	143 143	33.989 34.383	25.686 26.277	42.654 41.655	1.00	71.38
40	1154	Ň	GLU C	144	34.272	24.416	41.035	1.00 1.00	71.38 78.73
	1155	CA	GLU C	144	35.065	23.659	41.954	1.00	78.73 78.73
	1156	CB	GLU C	144	35.604	22,384	42.599	1.00	249.12
	1157	CG	GLU C	144	36.574	22.653	43.732	1.00	249.12
4.5	1158	CD	GLU C	144	36.019	22.238	45.078	1.00	249.12
45	1159	OE1	GLU C	144	35.711	21.040	45.239	1.00	249.12
	1160 1161	OE2	GLU C	144	35.889	23.102	45.972	1.00	249.12
	1162	C O	GLU C	144 144	34.222 34.767	23.316 22. 9 33	40.739	1.00	78.73
	1163	Ň	ASP C	145	32.898	23.473	39.711 40.853	1.00 1.00	78.73
50	1164	CA	ASP C	145	31.977	23.174	39.754	1.00	62.47 62.47
	1165	CB	ASP C	145	30.545	23.066	40.260	1.00	127.97
	1166	CG	ASP C	145	30.305	21.798	41.028	1.00	127.97
	1167	OD1	ASP C	145	30.493	20.714	40.441	1.00	127.97
55	1168	OD2	ASP C	145	29.935	21.883	42.217	1.00	127.97
55	1169	C	ASP C	145	32.053	24.220	38.663	1.00	62.47
	1170 1171	0 N	ASP C SER C	145	31.548	24.011	37.568	1.00	62.47
	1172	ČA	SER C	146 146	32.687 32.824	25.348	38.957	1.00	71.91
	1173	CB	SER C	146	33.438	26.397 27.641	37.960 38.599	1.00	71.91
60	1174	OG	SER C	146	32.599	28.127	39.630	1.00 1.00	151.98 151.98
	1175	C	SER C	146	33.711	25.866	36.837	1.00	71.91
	1176	0	SER C	146	34.648	25.109	37.082	1.00	71.91
	1177	N	GLY C	147	33.394	26.241	35.606	1.00	84.55
4 E	1178	CA	GLY C	147	34.170	25.785	34.466	1.00	84.55
65	1179	C	GLY C	147	33.449	26.062	33.158	1.00	84.55
	1180 1181	0 N	GLY C	147	32.552	26.898	33.121	1.00	84.55
	1182	CA	THR C	148 148	33.836 33.192	25.373 25.581	32.084	1.00	54.14
	1183	CB	THR C	148	34.166	25.561 26.153	30.781	1.00	54.14
70	1184	OG1	THR C	148	34.588	25.133	29.760 28.858	1.00 1.00	64.28
						20.100	20.000	1.00	64.28

	1185 1186 1187	CG2 C O	THR C THR C THR C	148 148	.35.394 32.671	26.717 24.216	30.474 30.285	1.00 1.00	64.28 54.14
5	1188 1189 1190	N CA CB	TYR C TYR C TYR C	148 149 149 149	33.429 31.359 30.725 29.524	23.287 24.119 22.879 22.656	30.032 30.145 29.753	1.00 1.00 1.00	54.14 33.05 33.05
	1191 1192 1193	CG CD1 CE1	TYR C TYR C TYR C	149 149 149	29.787 30.185 30.359	22.522 23.612 23.470	30.627 32.108 32.391 34.266	1.00 1.00 1.00 1.00	43.72 43.72 43.72
10	1194 1195 1196	CD2 CE2 CZ	TYR C TYR C TYR C	149 149 149	29.574 29.739 30.130	21.296 21.143 22.222	32.738 34.095 34.876	1.00 1.00 1.00	43.72 43.72 43.72 43.72
15	1197 1198 1199	OH C	TYR C TYR C TYR C	149 149 149	30.255 30.257 30.212	22.023 22.872 23.905	36.258 28.312 27.666	1.00 1.00 1.00	43.72 43.72 33.05 33.05
	1200 1201 1202 1203	N CA CB CG	TYR C TYR C TYR C	150 150 150	29.929 29.402 30.453	21.687 21.473 21.790	27.818 26.481 25.384	1.00 1.00 1.00	75.60 75.60 80.46
20	1204 1205 1206	CD1 CT: CD2	TYR C TYR C TYR C TYR C	150 150 150 150	31.554 31.282 32.288 32.874	20.780 19.581 18.664	25.087 24.439 24.162	1.00 1.00 1.00	80.46 80.46 80.46
25	1207 1208 1209	CE2 CZ OH	TYR C TYR C TYR C	150 150 150	33.889 33.590 34.597	21.039 20.130 18.938 18.011	25.445 25.168 24.529 24.280	1.00 1.00 1.00 1.00	80.46 80.46 80.46
	1210 1211 1212	C O N	TYR C TYR C CYS C	150 150 151	28.963 29.374 28.090	20.007 19.239 19.604	26.498 27.375 25.586	1.00 1.00 1.00	80.46 75.60 75.60 100.28
30	1213 1214 1215	CA C O	CYS C CYS C CYS C	151 151 151	27.657 27.674 27.634	18.211 17.617 18.349	25.572 24.167 23.191	1.00 1.00 1.00	100.28 100.28 100.28
35	1216 1217 1218 1219	CB SG N CA	CYS C CYS C THR C THR C	151 151 152	26.255 24.959 27.746	18.096 19.135 16.291	26.172 25.424 24.074	1.00 1.00 1.00	64.15 64.15 69.97
55	1220 1221 1222	CB OG1 CG2	THR C THR C THR C	152 152 152 152	27.755 29.089 29.210 30.247	15.598 14.837 13.780 15.771	22.795 22.588 23.550 22.765	1.00 1.00 1.00	69.97 86.22 86.22
40	1223 1224 1225	C O N	THR C THR C GLY C	152 152 153	26.594 26.242 25.992	14.610 14.082 14.368	22.813 23.879 21.652	1.00 1.00 1.00 1.00	86.22 69.97 69.97 96.14
45	1226 1227 1228	CA C O	GLY C GLY C	153 153 153	24.879 24.588 25.037	13.441 13.010 13.663	21.597 20.182 19.247	1.00 1.00 1.00	96.14 96.14 96.14
43	1229 1230 1231 1232	N CA CB CG	LYS C LYS C	154 154 154	23.845 23.522 23.722	11.918 11.431 9.916	20.017 18.690 18.603	1.00 1.00 1.00	77.66 77.66 222.01
50	1233 1234 1235	CD CE NZ	LYS C LYS C LYS C LYS C	154 154 154 154	23.538 23.820 23.556 23.726	9.323 7.833 7.151 5.689	17.212 17.253 15.924 16.075	1.00 1.00 1.00	222.01 222.01 222.01
	1236 1237 1238	C O N	LYS C LYS C VAL C	154 154 155	22.086 21.221 21.843	11.796 11.567 12.405	18.428 19.269 17.271	1.00 1.00 1.00 1.00	222.01 77.66 77.66 110.66
55	1239 1240 1241	CA CB CG1	VAL C VAL C VAL C	155 155 155	20.496 20.397 18.985	12.796 14.288 14.643	16.862 16.589 16.163	1.00 1.00 1.00	110.66 77.82 77.82
60	1242 1243 1244 1245	CG2 C O N	VAL C VAL C VAL C	155 155 155	20.778 20.208 21.000	15.046 12.046 12.085	17.834 15.579 14.629	1.00 1.00 1.00	77.82 110.66 110.66
	1246 1247 1248	CA CB CG	TRP C TRP C TRP C TRP C	156 156 156 156	19.074 18.727 18.811 17.823	11.363 10.560 11.362	15.553 14.401 13.120	1.00 1.00 1.00	192.10 192.10 246.44
65	1249 1250 1251	CD2 CE2 CE3	TRP C TRP C TRP C	156 156 156	16.417 15.830 15.592	12.399 12.222 13.503 11.100	13.086 13.206 13.150 13.355	1.00 1.00 1.00 1.00	246.44 246.44 246.44
70	1252 1253 1254	CD1 NE1 CZ2	TRP C TRP C TRP C	156 156 156	18.042 16.846 14.454	13.729 14.407 13.698	12.960 13.005 13.239	1.00 1.00 1.00 1.00	246.44 246.44 246.44 246.44

	1255 1256	CZ3 CH2	TRP C	156 156	· 14.217 13.662	11.293	13.438	1.00	248.44
	1257	C	TRP C	156	19.771	12.588 9.496	13.378 14.335	1.00	246.44
	1258	ŏ	TRP C	156	19.673	8.478	15.006	1.00 1.00	192.10
5	1259	N	GLN C	157	20.800	9.769	13.545	1.00	192.10
	1260	CA	GLN C	157	21.861	8.814	13.373	1.00	118.64 118.64
	1261	CB	GLN C	157	21.511	7.931	12.180	1.00	249.64
	1262	CG	GLN C	157	20.361	6.995	12.528	1.00	249.64
10	1263	CD	GLN C	157	20.670	6.255	13.803	1.00	249.64
10	1264 1265	OE1 NE2	GLN C GLN C	157	21.748	5.725	13.918	1.00	249.64
	1266	C	GLN C GLN C	157 157	19.770 23.230	6.241	14.761	1.00	249.64
	1267	ŏ	GLN C	157	24.183	9.430 8.768	13.234 12.826	1.00	118.64
	1268	Ň	LEU C	158	23.323	10.707	13.574	1.00 1.00	118.64 91.98
15	1269	CA	LEU C	158	24.600	11.404	13.510	1.00	91.98
	1270	CB	LEU C	158	24.580	12.461	12.418	1.00	164.15
	1271	CG	LEU C	158	24.775	11.991	10.980	1.00	164.15
	1272	CD1	LEU C	158	25.736	12.973	10.359	1.00	164.15
20	1273 1274	CD2 C	LEU C	158	25.383	10.614	10.868	1.00	164.15
~0	1275	ŏ	LEU C	158 158	25.000 24.147	12.046 12.397	14.841	1.00	91.98
	1276	Ň	ASP C	159	26.307	12.190	15.658 15.047	1.00	91.98
	1277	CA	ASP C	159	26.839	12.762	16.273	1.00 1.00	113.11
	1278	СВ	ASP C	159	28.230	12.173	16.564	1.00	113.11 249.37
25	1279	CG	ASP C	159	28.236	10.645	16.599	1.00	249.37
	1280	OD1	ASP C	159	27.536	10.057	17.451	1.00	249.37
	1281	OD2	ASP C	159	28.949	10.033	15.771	1.00	249.37
	1282 1283	C	ASP C	159	26.939	14.280	16.148	1.00	113.11
30	1284	O N	ASP C TYR C	159	27.223 26.701	14.788	15.063	1.00	113.11
30	1285	CA	TYR C	160 160	26.701	14.995 16.464	17.254	1.00	103.02
	1286	CB	TYR C	160	25.424	17.105	17 <i>.2</i> 78 17.057	1.00 1.00	103.02
	1287	CG	TYR C	160	24.711	16.622	15.826	1.00	177.48 177.48
~-	1288	CD1	TYR C	160	23.860	15.521	15.882	1.00	177.48
35	1289	CE1	TYR C	160	23.204	15.062	14.752	1.00	177.48
	1290	CD2	TYR C	160	24.891	17.255	14.600	1.00	177.48
	1291 1292	CE2	TYR C	160	24.241	16.804	13.458	1.00	177.48
	1293	CZ OH	TYR C	160	23.400	15.707	13.545	1.00	177.48
40	1294	C	TYR C	160 160	22.763 27.333	15.245 16.998	12.427	1.00	177.48
	1295	ŏ	TYR C	160	27.095	16.449	18.581 19.647	1.00	103.02
	1296	Ň	GLU C	161	28.052	18.102	18.474	1.00 1.00	103.02
	1297	CA	GLU C	161	28.687	18.775	19.599	1.00	74.72 74.72
4.5	1298	CB	GLU C	161	30.170	18.972	19.273	1.00	249.14
45	1299	cc	GLU C	161	30.978	19.729	20.300	1.00	249.14
	1300	CD	GLU C	161	32.456	19.531	20.085	1.00	249.14
	1301 1302	OE1 OE2	GLU C	161	33.259	20.350	20.582	1.00	249.14
	1302	C	GLU C	161	32.808	18.538	19.417	1.00	249.14
50	1304	ŏ	GLU C	161 161	27.985 27.656	20.117 20.780	19.779	1.00	74.72
	1305	Ň	SER C	162	27.743	20.780	18.806 21.021	1.00	74.72
	1306	CA	SER C	162	27.055	21.776	21.320	1.00 1.00	59.53 50.53
	1307	CB	SER C	162	26.210	21.627	22.573	1.00	59.53 71.52
F.F	1308	OG.	SER C	162	27.017	21.253	23.673	1.00	71.52 71.52
55	1309	Ç	SER C	162	28.038	22.914	21.532	1.00	59.53
	1310	O.	SER C	162	29.247	22.679	21.608	1.00	59.53
	1311 1312	N CA	GLU C	163	27.521	24.145	21.615	1.00	68.20
	1313	CB	GLU C	163 163	28.371	25.330	21.810	1.00	68.20
60	1314	čĠ	GLU C	163	27.580 27.289	26.610 26.902	21.565	1.00	172.64
	1315	CD	GLU C	163	28.513	27.375	20.098 19.334	1.00	172.64 172.64
	1316	OE1	GLU C	163	29.120	28.383	19.757	1.00 1.00	172.64
	1317	OE2	GLU C	163	28.864	26.748	18.311	1.00	172.64
<i>C</i> =	1318	Č	GLU C	163	28.856	25.296	23.246	1.00	68.20
65	1319	0	GLU C	163	28.104	24.920	24.131	1.00	68.20
	1320 1321	N	PRO C	164	30.123	25.683	23.498	1.00	54.78
	1321	CD CA	PRO C	164	31.163	26.188	22.601	1.00	96.83
	1323	CB	PRO C PRO C	164 164	30.609	25.645 06.854	24.876	1.00	54.78
70	1324	CG	PRO C	164	32.109 32.176	25.851 26.765	24.709 23.584	1.00	96.83
						20.703	23.584	1.00	96.83

	1325	C	PRO C	164	- 29.950	26.720	25.688	1.00	54.78
	1326 1327	. 0	PRO C	164	29.480	27.695	25.137	1.00	54.78
	1328	· N CA	LEU C	165 165	29.898 29.272	26.537 27.513	27.000	1.00	73.43
5	1329	CB	LEU C	165	27.829	27.513 27.112	27.861 28.127	1.00 1.00	73.43
	1330	CG	LEU C	165	27.163	27.955	29.201	1.00	54.02 54.02
	1331	CD1	LEU C	165	27.395	29.384	28.820	1.00	54.02
	1332	CD2	LEU C	165	25.690	27.66 5	29.329	1.00	54.02
10	1333 1334	C	LEU C	165	30.010	27.634	29.164	1.00	73.43
10	1335	N	LEU C	165 166	30.200 30.420	26.641 28.853	29.859 29.493	1.00	73.43
	1336	ČA	ASN C	166	31.148	29.098	30.736	1.00 1.00	53.84
	1337	CB	ASN C	166	31.979	30.368	30.646	1.00	53.84 80.99
1.5	1338	CG	ASN C	166	33.392	30.110	30.181	1.00	80.99
15	1339	OD1	ASN C	166	33.956	29.054	30.431	1.00	80.99
	1340 1341	ND2 C	ASN C	166	33.973	31.096	29.516	1.00	80.99
	1342	Ö	ASN C	166 166	30.233 29.145	29.236	31.918	1.00	53.84
	1343	Ň	ILE C	167	30.693	29.756 28.806	31.789 33.084	1.00 1.00	53.84
20	1344	CA	ILE C	167	29.878	28.881	34,292	1.00	65.33 65.33
	1345	CB	ILE C	167	29.218	27.527	34.603	1.00	38.60
	1346	CG2	ILE C	167	28.736	27.503	36.027	1.00	38.60
	1347 1348	CG1	ILE C	167	28.066	27.269	33.618	1.00	38.60
25	1349	CD1 C	ILE C	167 167	27.261 30.717	26.070	33.933	1.00	38.60
23	1350	ŏ	ILE C	167	31.781	29.258 28.681	35.475 35.694	1.00 1.00	65.33
	1351	Ň	THR C	168	30.1.10	30.223	36.246	1.00	65.33 58.90
	1352	CA	THR C	168	31.015	30.619	37.406	1.00	58.90
20	1353	CB	THR C	168	31.537	32.023	37.260	1.00	100.28
30	1354	OG1	THR C	168	32.315	32.110	36.067	1.00	100.28
	1355 1356	CG2 C	THR C	168	32.406	32.354	38.4 3 8	1.00	100.28
	1357	ŏ	THR C	168 168	30.230 29.042	30.502 30.852	38.708 38.795	1.00	58.90
	1358	Ň	VAL C	169	30.908	29.965	39.708	1.00 1.00	58.90 74.23
35	1359	CA	VAL C	169	30.337	29.795	41.021	1.00	74.23
	1360	CB	VAL C	169	30.424	28.330	41.467	1.00	86.72
	1361	CG1	VAL C	169	30.314	28.229	42.962	1.00	86.72
	1362 1363	CG2 C	VAL C	169 169	29.323	27.547	40.813	1.00	86.72
40	1364	ŏ	VAL C	169	31.196 32.359	30.668 30.328	41.924 42.184	1.00 1.00	74.23
	1365	Ň	ILE C	170	30.645	31.805	42.365	1.00	74.23 66.08
	1366	CA	ILE C	170	31.376	32.711	43.252	1.00	66.08
	1367	CB	ILE C	170	30.995	34.166	42.997	1.00	82.85
45	1368 1369	CG2	ILE C	170	31.079	34.476	41.520	1.00	82.85
43	1370	CG1 CD1	ILE C	170 170	29.572 29.097	34.412	43.431	1.00	82.85
	1371	C.	ILL C	170	31.092	35.848 32.355	43.156 44.701	1.00 1.00	82.85 66.08
	1372	Ö	ILE C	170	30.272	31.482	44.960	1.00	66.08
<i></i> 0	1373	N	LYS C	171	31.771	32.999	45.644	1.00	110.58
50	1374	CA	LYS C	171	31.545	32.688	47.052	1.00	110.58
	1375 1376	CB	LYS C	171	32.749	31.935	47.625	1.00	192.81
	1377	CD	LYS C	171 171	34.062 35.247	32.679	47.478	1.00	192.81
	1378	CE	LYS C	171	35.319	31. 72 3 30.934	47.505 48.803	1.00	102.81 192.81
55	1379	NZ	LYS C	171	36.464	29.978	48.796	1.00	192.81
	1380	C	LYS C	171	31.263	33.931	47.882	1.00	110.58
	1381	0	LY3 C	171	30.884	33.830	49.050	1.00	110.58
	1382 1383	C1	NAG C	221	4.609	28.125	21.539	1.00	246.09
60	1384	C2 N2	NAG C NAG C	221 221	4.738	26.611	21.473	1.00	248.09
•••	1385	C7	NAG C	221	6.129 6.578	26.254 25.075	21.269 21.680	1.00 1.00	248.09 248.09
	1386	07	NAG C	221	5.867	24.254	22.257	1.00	248.09
	1387	C8	NAG C	221	8.042	24.762	21.420	1.00	248.09
65	1388	C3	NAG C	221	3.908	26.047	20.327	1.00	248.09
(J)	1389 1390	03 C4	NAG C	221	3.902	24.630	20.401	1.00	248.09
	1390	04	NAG C	221 221	2.465 1.852	26.559	20.341	1.00	248.09
	1392	C5	NAG C	221	2.447	26.163 28.0 9 6	19.095 20.488	1.00 1.00	248.09
	1393	05	NAG C	221	3.226	28.499	21.641	1.00	248.09 248.09
70	1394	C6	NAG C	221	1.052	28.659	20.692	1.00	248.09

	1395	O 6	NAG C	221	- 0.460	28.142	21.875	1.00	242.22
	1396	C1	NAG C	222	0.468	26,179	18.986	1.00	248.09
	1397	C2	NAG C	222	-0.014	24.897	18.283	1.00	248.99
	1398	N2	NAG C	222	0.382	23.729	19.048	1.00	248.99
5	1399	C7	NAG C	222	-0.541	22.909	19.543	1.00	248.99
•	1400	07	NAG C	222	-1.750	23.088	19.392	1.00	248.99
	1401	C8	NAG C	222	-0.046	21.704	20.330	1.00	248.99
	1402	čš	NAG C	222	0.566	24.815	16.861	1.00	248.99
	1403	03	NAG C	222	-0.012	23.714	16.171	1.00 1.00	248.99
10	1404	C4	NAG C	222	0.292	26.112	16.083	1.00	248.99
	1405	04	NAG C	222	0.989	26.082	14.843	1.00	248.99
	1406	C5	NAG C	222	0.742	27.337	16.897	1.00	248.99
	1407	O5	NAG C	222	0.107	27.330	18.201	1.00	248.99
	1408	C6	NAG C	222	0.396	28.661	16.232	1.00	248.99
15	1409	O 6	NAG C	222	1.499	29.556	16.260	1.00	248.99
	1410	C1	NAG C	242	18.858	43.706	21.097	1.00	248.99
	1411	C2	NAG C	242	18.159	43.460	19.760	1.00	98.91 98.91
	1412	N2	NAG C	242	16.728	43.568	19.914	1.00	98.91
	1413	C7	NAG C	242	16.062	44.435	19.166	1.00	98.91
20	1414	07	NAG C	242	16.610	45.163	18.336	1.00	98.91
	1415	C8	NAG C	242	14.561	44.512	19.366	1.00	98.91
	1416	C3	NAG C	242	18.507	42.075	19.237	1.00	98.91
	1417	O3	NAG C	242	17.925	41.880	17.955	1.00	98.91
	1418	C4	NAG C	242	20.020	41.925	19.144	1.00	98.91
25	1419	04	NAG C	242	20.340	40.556	18.833	1.00	98.91
	1420	C5	NAG C	242	20.708	42.318	20.459	1.00	98.91
	1421	O 5	NAG C	242	20.270	43.615	20.916	1.00	98.91
	1422	C6	NAG C	242	22.196	42.434	20.243	1.00	98.91
	1423	O6	NAG C	242	22.917	41.643	21,170	1.00	98.91
30	1424	C1	NAG C	243	20.966	40.334	17.621	1.00	148.54
	1425	C2	NAG C	243	21.805	39.050	17.674	1.00	148.54
	1426	N2	NAG C	243	22.863	39.159	18.662	1.00	148.54
	1427	C7	NAG C	243	23.081	38.154	19.504	1.00	148.54
25	1428	07	NAG C	243	22.402	37.126	19.506 ·	1.00	148.54
35	1429	C8	NAG C	243	24.212	38.320	20.503	1.00	148.54
	1430	. C3	NAG C	243	22.422	38.803	16.299	1.00	148.54
	1431	03	NAG C	243	23.126	37.573	16.300	1.00	148.54
	1432	C4	NAG C	243	21.341	38.791	15.201	1.00	148.54
40	1433	04	NAG C	243	21.974	38.713	13.890	1.00	148.54
40	1434	C5	NAG C	243	20.529	40.090	15.296	1.00	148.54
	1435	O5	NAG C	243	19.954	40.216	16.611	1.00	148.54
	1436	C6	NAG C	243	19.402	40.197	14.299	1.00	148.54
	1437 1438	O6	NAG C	243	18.380	39.264	14.597	1.00	148.54
45	1439	C1	MAN C	244	21.585	37.818	12.938	1.00	182.20
73	1440	C2 C2	MAN C MAN C	244	21.654	36.312	13.272	1.00	182.20
	1441	C3	MAN C	244	20.383	35.858	13.660	1.00	182.20
	1442	og Og	MAN C	244 244	22.042	35.694	11.892	1.00	182.20
	1443	∝	MAN C	244	22.157 21.095	34.284 36.131	11.945	1.00	182.20
50	1444	ŏ4	MAN C	244	21.095 1.496	35.520	10.730	1.00	182.20
-	1445	Č5	MAN C	244	∠1.199	37. 66 6	9.503 10.607	1.00 1.00	182.20
	1446	O5	MAN C	244	20.771	38.312	11.834		182.20
	1447	Č6	MAN C	244	20.464	38.264	9.406	1.00 1.00	182.20 182.20
	1448	06	MAN C	244	19.092	38.434	9.670	1.00	
55	1449	C1	NAG C	250	-1.001	38.689	31.557	1.00	182.20
	1450	C2	NAG C	250	-1.761	€ 27.609	32.354	1.00	249.77 249.77
	1451	N2	NAG C	250	-1.602	37.821	33.782	1.00	249.77
	1452	C7	NAG C	250	-2.636	38.209	34.526	1.00	249.77
	1453	07	NAG C	250	-3.761	38.414	34.060	1.00	249.77
60	1454	C8	NAG C	250	-2.384	38.404	36.016	1.00	249.77
	1455	cs	NAG C	250	-1.221	36.224	31.975	1.00	249.77
	1456	03	NAG C	250	-1.975	35.209	32. 62 6	1.00	249.77
	1457	C4	NAG C	250	-1.287	36.028	30.458	1.00	249.77
	1458	04	NAG C	250	-0.662	34.799	30.113	1.00	249.77
65	1459	C5	NAG C	250	-0.582	37.194	29.736	1.00	249.77
	1460	O5	NAG C	250	-1.150	38.457	30.150	1.00	249.77
	1461	Ç6	NAG C	250	-0.717	37.121	28.224	1.00	249.77
	1482	O6	NAG C	250	-0.351	38.351	27.612	1.00	249.77
70	1463	C1	NAG C	274	16.034	53.837	43.921	1.00	248.46
70	1464	C2	NAG C	274	17.088	53.346	44.921	1.00	248.46

	1485	N2	NAG C	274	. 16.465	52.511	45.928	1.00	248.46
	1466	C7	NAG C	274	17.189	51.604	46.575	1.00	248.46
∵.	1487	07	NAG C	274	18.387	51.422	46.354	1.00	248.46
5	1468	C8	NAG C	274	16.474	50.767	47.625	1.00	248.46
3	1469 1470	C3 O3	NAG C	274	17.768	54.539	45.598	1.00	248.46
	1471	3 3	NAG C NAG C	274 274	18.835	54.081	46.416	1.00	248.46
•	1472	3	NAG C	274	18.306 18.793	55.518 56.685	44.553 45.202	1.00	248.46
	1473	C5	NAG C	274	17.195	55.898	43.563	1.00 1.00	248.46
10	1474	O5	NAG C	274	16.641	54.710	42.959	1.00	248.46 248.46
	1475	C6	NAG C	274	17.688	56.784	42.432	1.00	248.46
	1476	O6	NAG C	274	16.703	56.920	41.418	1.00	248.46
	1477 1478	C1	NAG C	335	15.450	18.012	31.039	1.00	249.77
15	1479	C2 N2	NAG C NAG C	335 335	14.351 14.844	18.418	72.049	1.00	249.77
~~	1480	C7	NAG C	335	15.027	18.144 19.131	3.1. 387 34. 25 8	1.00	249.77
	1481	07	NAG C	335	14.782	20.312	34.004	1.00 1.00	249.77
	1482	C8	NAG C	335	15.555	18.743	35.627	1.00	249.77 249.77
20	1483	C3	NAG C	335	13.010	17.686	31.860	1.00	249.77
20	1484	O3	NAG C	335	11.981	18.411	32.519	1.00	249.77
	1485 1486	C4 O4	NAG C	335	12.654	17.546	30.386	1.00	249.77
	1487	C5	NAG C NAG C	335 335	11.455 13.801	16.796	30.245	1.00	249.77
	1488	O5	NAG C	335	14.974	16.839 17.683	29.679 29.710	1.00 1.00	249.77
25	1489	C6	NAG C	335	13.481	16.566	28.214	1.00	249.77 249.77
	1490	O6	NAG C	335	13.512	15.176	27.922	1.00	249.77
	1491	C1	NAG C	340	26.860	22.059	50.969	1.00	249.77
	1492	C2	NAG C	340	27.612	23.165	51.681	1.00	249.77
30	1493 1494	N2 C7	NAG C NAG C	340	28.257	24.040	50.724	1.00	243.77
50	1495	07	NAG C	340 340	28.068 27.368	25.353 25.865	50.821	1.00	249.77
	1496	Č8	NAG C	340	28.755	26.232	51.703 49.794	1.00 1.00	249.77
	1497	C3	NAG C	340	28.630	22.560	52.634	1.00	249.77 249.77
25	1498	03	NAG C	340	29.275	23.608	53.354	1.00	249.77
35	1499	C4	NAG C	340	27.915	21.620	53.612	1.00	249.77
	1500 1501	O4 C5	NAG C	340	28.896	20.922	54. 36 5	1.00	249.77
	1502	O5	NAG C NAG C	340 340	26.987 26.141	20.611	52.880	1.00	249.77
	1503	C6	NAG C	340	26.045	21.281 19.869	51.923 53.817	1.00 1.00	249.77
40	1504	O6	NAG C	340	24.805	19.571	53.193	1.00	249.77 249.77
	1505	C1	NAG C	366	35.293	30.923	28.965	1.00	158.36
	1506	C2	NAG C	366	35.391	31.732	27.687	1.00	158.36
	1507 1508	N2 C7	NAG C	366	34.394	31.261	26.748	1.00	158.36
45	1509	07 07	NAG C NAG C	366 366	33,197 32.885	31.835	26.713	1.00	158.36
	1510	C8	NAG C	366	32.191	32.778 31.285	27.446 25.707	1.00 1.00	158.36
	1511	C3	NAG C	366	36.780	31.584	27.089	1.00	158.36 158.36
	1512	03	NAG C	366	36.910	32.481	25.981	1.00	158.36
50	1513	C4	NAG C	366	37.866	31.903	28.119	1.00	158.56
50	1514 1515	04 05	NAG C	366	39.144	31.523	27.573	1.00	158.36
	1516	C5 O5	NAG C NAG C	366 366	37.620	31.138	29.429	1.00	158.36
	1517	C6	NAG C	366	36.277 38.550	31.367 31.570	29.896	1.00	158.36
	1518	06	NAG C	366	38.325	31.570 30.807	30.549 31. 72 7	1.00 1.00	158.36
55	1519	C1	NAG C	367	40.136	32.494	27.559	1.00	158.36 249.59
	1520	C2	NAG C	367	41.511	31.828	27.487	1.00	249.59
	1521	N2	NAG C	367	41.702	30.834	28.613	1.00	249.58
	1522 1523	C7 O7	NAG C	367	41.695	29.619	28.418	1.00	249.59
60	1524	C8	NAG C NAG C	367 367	41.532 41.899	29.106	27.308	1.00	249.59
	1525	C3	NAG C	367	42.590	28.735 32.914	29.639 27.465	1.00	249.59
	1526	03	NAG C	367	43.877	32.321	27.352	1.00	249.59 249.59
	1527	C4	NAG C	367	42.343	33.850	26.278	1.00	249,59
65	1528	O4	NAG C	367	43.281	34.917	26.303	1.00	249.59
O)	1529 1530	C5 O5	NAG C	367	40.913	34.411	26.335	1.00	249.59
	1531	C6	NAG C NAG C	367 367	39.945	33.331	26.405	1.00	249.59
	1532	06	NAG C	367 367	40.576 39.610	35.245 34.604	25.112	1.00	249.59
	1533	CB	LYS A	4	5.822	17.052	24.292 16.197	1.00 1.00	249.59
70	1534	ca	LYS A	4	4.918	18.220	15.853	1.00	225.85 225.85

	1535	CD	LYS A	4	4.535	18.995	17 100	4.00	
	1536	CE	LYS A	4	3.638	20.173	17.100 16.766	1.00	225.85
	1537	NZ	LYS A	4	3.267	20.934	17.987	1.00	225.85
	1538	C	LYS A	4	7.001	17.239	14.016	1.00	225.85
5	1539	ō	LYS A	4	7.491	18.292	14.419	1.00	249.21
	1540	Ň	LYS A	4	7.236	15.183	15.408	1.00	249.21
	1541	CA	LYS A	4	6.316	16.275	14.978	1.00	249.21
	1542	N	PRO A	5	7.053	- 16.880	12.723	1.00	249.21
	1543	CD	PRO A	5	6.773	15.535	12.187	1.00	94.49
10	1544	CA	PRO A	5	7.685	17.735	11.709	1.00	84.99
	1545	СВ	PRO A	5	8.092	16.736	10.629	1.00	94.49
	1546	CG	PRO A	5	7.010	15.716	10.691	1.00	84.99
	1547	C	PRO A	5	6.772	18.825	11.164	1.00	84.99
	1548	Ō	PRO A	5	5.557	18.721	11.227	1.00	94.49
15	1549	N	LYS A	6	7.358	19.877	10.617	1.00	94.49
	1550	CA	LYS A	6	6.559	20.973	10.017	1.00 1.00	99.70
	155 i	СВ	LYS A	6	6.444	22.094	11.130	1.00	99.70
	1552	CG	LYS A	6	5.540	23.242	10.711	1.00	128.86
	1553	CD	LYS A	6	5.290	24.223	11.853	1.00	128.86
20	1554	CE	LYS A	6	4.321	25.329	11.418	1.00	128.86
	1555	NZ	LYS A	6	3.977	26.285	12.517	1.00	128.86
	1556	С	LYS A	6	7.166	21.512	8.793	1.00	128.86
	1557	0	LYS A	6	8.281	22.029	8.801	1.00	99.70
	1558	N	VAL A	7	6.421	21.395	7.693	1.00	99.70
25 ·	. 1559	CA	VAL A	7	6.878	21.852	6.377	1.00	71.19
	1560	CB	VAL. A	7	5.955	21.392	5.243	1.00	71.19 54.73
	1561	CG1	VAL A	7	6.584	21.739	3.900	1.00	54.73 54.73
	1562	CG2	VAL A	7	5.687	19.922	5.350	1.00	54.73
	1563	С	VAL A	7	6.947	23.354	6.221	1.00	71.19
30	1564	0	VAL A	7	5.924	24.023	6.282	1.00	71.19
	1565	N	SER A	8	8.141	23.885	5.988	1.00	76.52
	1566	CA	SER A	8	8.301	25.325	5.804	1.00	76.52
	1567	CB	SER A	8	9.537	25.827	6.563	1.00	232.80
25	1568	OG.	SER A	8	10.701	25.106	6.196	1.00	232.80
35	1569	Ç	SER A	8	8.437	25.597	4.311	1.00	76.52
	1570	0	SER A	8	8.665	24.679	3.534	1.00	76.52
	1571	N	LEU A	9	8.274	26.851	3.914	1.00	77.48
	1572	CA	LEU A	9	8.388	27.237	2.509	1.00	77.48
40	1573	CB	LEU A	9	7.037	27.651	1.935	1.00	70.08
40	1574	cg	LEU A	9	5.879	26.663	1.868	1.00	70.08
	1575	CD1	LEU A	9	4.901	27.105	0.816	1.00	70.08
	1576	CD2	LEU A	9	6.399	25.305	1.517	1.00	70.08
	1577 1578	C 0 ·	LEU A	9	9.321	28.417	2.334	1.00	77.48
45	1579	N	LEU A	9	9.506	29.212	3.257	1.00	77.48
75	1580	CA	ASN A ASN A	10	9.896	28.544	1.140	1.00	96.41
	1581	CB	ASN A	10	10.795	29.657	0.844	1.00	96.41
	1582	CG	ASN A	10	12.196	29.384	1.384	1.00	121.54
	1583	OD1	ASN A	10	13.074	30.616	1.338	1.00	121.54
50	1584	ND2	ASN A	10	12.819	31.598	2.041	1.00	121.54
	1585	C	ASN A	10 10	14.108	30.581	0.496	1.00	121.54
	1586	ŏ	ASN A	10	10.868 11.396	29.920	-0.654	1.00	96.41
	1587	Ň	PRO A	11	10.325	29.110	-1.412	1.00	96.41
	1588	CD	PRO A	11		31.064	-1.105	1.00	78.36
55	1589	CA	PRO A	11	10.263	31.320	-2.548	1.00	72.21
	1590	CB	PRO A	11	9.642 9.130	32.128	-0.350	1.00	78.36
	1591	ČĞ	PRO A	11	10.084	33.049	-1.455	1.00	72.21
	1592	Č	PRO A	11	8.492	32.803	-2.583	1.00	72.21
	1593	ŏ	PRO A	11	7.992	31.647 30.537	0.551	1.00	78.36
60	1594	N	PRO A	12	8.056	32.469	0.386	1.00	78.36
	1595	CD	PRO A	12	8.570	33.812	1.513	1.00	81.66
	1596	CA	PRO A	12	6.968	32.110	1.833 2.430	1.00	122.93
	1597	CB	PRO A	12	6.925	33.274		1.00	81.66
	1598	CG	PRO A	12	8.277	33.895	3.409 3.290	1.00	122.93
65	1599	С	PRO A	12	5.637	31.998	1. 663	1.00	122.93
	1600	0	PRO A	12	4.695	31.307	2.081	1.00	81.66
	1601	N	TRP A	13	5.579	32.699	0.538	1.00 1.00	81.66
	1602	CA	TRP A	13	4.388	32.725	-0.293	1.00	66.49
70	1603	CB	TRP A	13	4.660	33.539	-1.562	1.00	66.49
70	1604	CG	TRP A	13	5.336	34.831	-1.277	1.00	100.34 100.34
								1.00	100.34

	1605	CD2	TRP A	13	· 5.100	35.697	-0.167	1.00	100.04
	1606	CE2	TRP A	13	6.000	36.762	-0.268	1.00 1.00	100.34 100.34
	1607	CE3	TRP A	13	4.210	35.673	0.909	1.00	100.34
5	1608	CD1	TRP A	13	6.339	35.393	-1.9 96	1.00	100.34
3	1609 1610	NE1 CZ2	TRP A	13 13	6.748 6.046	36.552 37.795	-1.395 0.664	1.00	100.34
	1611	CZ3	TRP A	13	4.253	38.698	1.829	1.00 1.00	100.34 100.34
	1612	CH2	TRP A	13	5.167	37.745	1.705	1.00	100.34
10	1613	C	TRP A	13 -	3.913	31.342	-0.666	1.00	66.49
10	1614 1615	O N	TRP A ASN A	13 14	4.637	30.573	-1.270	1.00	66.49
	1616	CA	ASN A	14	2.685 2.109	31.031 29.738	-0.299 -0.629	1.00 1.00	52.07
	1617	CB	ASN A	14	1.508	29.082	0.626	1.00	52.07 104.36
1.5	1618	CG	ASN A	14	0.274	29.801	1.152	1.00	104.36
15	1619 1620	OD1 ND2	ASN A	14	0.305	31.001	1.465	1.00	104.36
	1621	C	ASN A ASN A	14 14	-0.822 1.056	29.058 29.792	1.269 -1.759	1.00 1.00	104.36
	1622	ŏ	ASN A	14	0.271	28.850	-1.928	1.00	52.07 52.07
20	1623	N	ARG A	15	1.026	30.900	-2.509	1.00	52.98
20	1624	CA	ARG A	15	0.131	31.078	-3.667	1.00	52.98
	1625 1626 .	CB	ARG A ARG A	15 15	-0.942 -1.533	32.109 32.043	-3.415 -2.077	1.00	66.97
	1627	CD	ARG A	15	-2.626	33.064	-2.077 -2.014	1.00 1.00	66.97 66.97
۰.	1628	NE	ARG A	15	-3.768	32.699	-2.837	1.00	66.97
25	1629	CZ	ARG A	15	-4.589	33.596	-3.363	1.00	66.97
	1630 1631	NH1 NH2	ARG A ARG A	15 15	-4.370 -5.629	34.890	-3.150	1.00	66.97
	1632	C	ARG A	15	1.080	33.213 31.659	-4.091 -4.687	1.00 1.00	66.97 52.98
••	1633	0	ARG A	15	1.510	32.817	-4.563	1.00	52.98
30	1634	N	ILE A	16	1.431	30.867	-5.684	1.00	61.11
	1635 1636	CA CB	ILE A	16	2.362	31.362	-6.667	1.00	61.11
	1637	CG2	ILE A	16 16	3.662 4.375	30.595 30.856	-6.632 -5.312	1.00 1.00	64.67
	1638	CG1	ILE A	16	3.385	29.117	-6.833	1.00	64.67 64.67
35	1639	CD1	ILE A	16	4.626	28.268	-6. 76 8	1.00	64.67
	1640 1641	C	ILE A	16	1.849	31.311	-8.070	1.00	61.11
	1842	N	ILE A PHE A	16 17	0.851 2.560	30.662 32.019	-8.361 -8.933	1.00 1.00	61.11
	1643	CA	PHE A	17	2.266	32.130	-10.348	1.00	81.85 81.85
40	1644	СВ	PHE A	17	2.902	33.411	-10.856	1.00	58.17
	1645 1646	CG CD1	PHE A	17	2.014	34.604	-10.777	1.00	58.17
	1647	CD2	PHE A PHE A	17 17	2.531 0.681	35.841 34.512	-10.422 -11.181	1.00 1.00	58.17
	1648	CE1	PHE A	17	1.751	36.965	-10.467	1.00	58.17 58.17
45	1649	CE2	PHE A	17	-0.125	35.639	-11.238	1.00	58.17
	1650 1651	cz	PHE A	17	0.415	36.876	-10.885	1.00	58.17
	1652	C	PHE A PHE A	17 17	2.851 3.749	30.940 30.259	-11.110 -10. 62 1	1.00	81.85
	1653	Ň	LYS A	18	2.353	30.699	-10.021	1.00 1.00	81.85 81.40
50	1654	CA	LYS A	18	2.842	29.602	-13.129	1.00	81.40
	1655	CB CC	LYS A	18	1.981	29.497	-14.385	1.00	133.55
	1656 1657	CG CD	LYS A LYS A	18 18	2.281 1.153	28.313 28.136	-15.277	1.00	133.55
	1658	CE	LYS A	18	1.389	26.136 26.957	-16.287 -17.216	1.00 1.00	133.55 133.55
55	1659	NZ.	LYS A	18	2.627	27.139	-18.030	1.00	133.55
	1660	C	LYS A	18	4.305	29.838	-13.515	1.00	81,40
	1661 1662	0 N	LYS A GLY A	18 19	4.683 5.141	30.921	-13.972	1.00	81.40
	1663	CA	GLY A	19	6.524	28.834 28.975	-13.313 -13.702	1.00 1.00	92.32 92.32
60	1664	C	GLY A	19	7.492	29.428	-12.643	1.00	92.32
	1665	o	GLY A	19	8.697	29.398	-12.866	1.00	92.32
	1666 1667	N CA	GLU A	20 20	6.996	29.853	-11.491	1.00	67.13
	1668	CB	GLU A	20	7.896 7.153	30.300 31.239	-10.422 -9.477	1.00 1.00	67.13
65	1669	CG	GLU A	20	6.439	32.361	-10.221	1.00	115.51 115.51
	1670	CD	GLU A	20	5.794	33.361	-9.300	1.00	115.51
	1671	OE1 OE2	GLU A	20	4.991	32.949	-8.432	1.00	115.51
	1672 1673	C C	GLU A GLU A	20 20	6.091 8.469	34.561 29.094	-9.454 -0.653	1.00	115.51
70	1874	ŏ	GLU A	20	8.035	29.094 27.953	-9.652 -9.861	1.00 1.00	67.13 67.13
				=	,		J.001	1.50	37.13

	1675	N	ASN A	21	9.456	29.329	-8.788	1.00	81.05
	1676	CA	ASN A	21	10.059	28.225	-8.040	1.00	81.05
	1677	CB	ASN A	21	11.562	28.078	-8.328	1.00	110.52
5	1678 1679	CG OD1	ASN A	21	11.923	28.283	-9.788	1.00	110.52
,	1680	ND2	ASN A	21 21	11.250 13.025	27.808	-10.699	1.00	110.52
	1681	C	ASN A	21	9.915	28.989 28.409	-9.995 -6.547	1.00	110.52
	1682	ŏ	ASN A	21	10.054	29.521	-6.035	1.00 1.00	81.05
	1683	N	VAL A	22	9.681	27.306	-5.848	1.00	81.05 79.17
10	1684	CA	VAL A	22	9.525	27.341	-4.404	1.00	79.17
	1685	CB	VAL A	22	8.057	27.304	-4.012	1.00	85.34
	1686 1687	CG1 CG2	VAL A	22	7.431	26.001	-4.486	1.00	85.34
	1688	C	VAL A	22 22	7.925 10.194	27.449	<i>-</i> 2.510	1.00	85.34
15	1689	ŏ	VAL A	22	10.194	26.117 25.070	-3.815 -4.469	1.00	79.17
	1690	Ň	THR A	23	10.676	26.240	-2.579	1.00 1.00	79.17 92.04
	1691	CA	THR A	23	11.367	25.145	-1.908	1.00	92.04
	1692	CB	THR A	23	12.775	25.585	-1.556	1.00	153.40
20	1693	OG1	THR A	23	13.414	26.089	-2.736	1.00	153.40
20	1694 1695	CG2 C	THR A	23	13.567	24.428	-0.993	1.00	153.40
	1696	Ö	THR A	23 23	10.667 10.364	24.698 25.525	-0.634	1.00	92.04
	1697	Ň	LEU A	24	10.403	23.404	0.212 -0.485	1.00 1.00	92.04 64.92
	1698	CA	LEU A	24	9.742	22.945	0.730	1.00	64.92
25	1699	CB	LEU A	24	8.564	22.015	0.427	1.00	83.07
	1700	CG	LEU A	24	7.676	22.301	-0.774	1.00	83.07
	1701	CD1	LEU A	24	6.400	21.482	-0.676	1.00	83.07
	1702 1703	CD2 C	LEU A LEU A	24 24	7.348 10.701	23.745	-0.837	1.00	83.07
30	1704	ŏ	LEU A	24	11.034	22.206 21.049	1.657 1.433	1.00	64.92
	1705	Ň	THR A	25	11.125	22.863	2.725	1.00 1.00	64.92 60.46
	1706	CA	THR A	25	12.026	22.227	3.665	1.00	60.46
	1707	CB	THR A	25	12.890	23.286	4.309	1.00	96.68
35	1708	OG1	THR A	25	13.523	24.040	3.273	1.00	96.68
33	1709 1710	CG2 C	THR A	25 25	13.943	22.654	5.175	1.00	96.68
	1711	ŏ	THR A	25 25	11.264 10.270	21.446 21.923	4.746 5.293	1.00	60.46
	1712	Ň	CYS A	26	11.717	20.239	5.293 5.048	1.00 1.00	60.46 126.10
40	1713	CA	CYS A	26	11.060	19.464	6.081	1.00	126.10
40	1714	Ç	CYS A	26	11.617	19.884	7.421	1.00	126.10
	1715	0	CYS A	26	12.813	20.108	7.566	1.00	126.10
	1716 1717	CB SG	CYS A	26	11.293	17.971	5.888	1.00	188.87
	1718	N N	ASN A	26 27	10.283 10.727	16.954 19.999	7.005 8.393	1.00	188.87
45	1719	CA	ASN A	27	11.065	20.379	9.747	1.00 1.00	248.12 248.12
	1720	CB	ASN 4	27	10.474	19.354	10.685	1.00	249.30
	1721	CG	ASN A	27	10.331	19.883	12.046	1.00	249.30
	1722	OD1	ASN A	27	9.999	21.050	12.192	1.00	249.30
50	1723 1724	ND2 C	ASN A ASN A	27	10.582	19.060	13.069	1.00	249.30
50	1725	ŏ	ASN A	27 27	12.549 13.220	20.546 19.591	10.040	1.00	248.12
	1726	Ň	GLY A	28	13.058	21.754	10.431 9.840	1.00 1.00	248.12
	1727	CA	GLY A	28	14.469	22.013	10.073	1.00	150.98 150.98
	1728	Ç	GLY A	28	14.771	23.413	9.596	1.00	150.98
55	1729	0	GLY A	28	14.541	23.731	8.435	1.00	150.98
	1730 1731	N CA	ASN A	29	15.288	24.258	10.480	1.00	168.28
	1732	CA CB	ASN A ASN A	29 29	15.576 15.714	638.نب	10.111	1.00	168.28
	1733	čĠ	ASN A	29	15.723	26.494 27.979	11.374 11.072	1.00	185.34
60	1734	OD1	ASN A	29	15.387	28.400	9.966	1.00 1.00	185.34 185.34
	1735	ND2	ASN A	29	16.097	28.782	12.059	1.00	185.34
	1736	C	ASN A	29	16.799	25.839	9.208	1.00	168.28
	1737	0	ASN A	29	16.704	26.492	8.165	1.00	168.28
65	1738 1739	N CA	ASN A ASN A	30	17.943	25.279 25.452	9.594	1.00	244.43
U	1740	CB	ASN A	30 30	19.151 20.131	25.453 26.363	8.797	1.00	244.43
	1741	ČĠ	ASN A	30	19.592	27.765	9.543 9.735	1.00 1.00	249.25 249.25
	1742	OD1	ASN A	30	19.601	28.297	10.843	1.00	249.25 249.25
70	1743	ND2	ASN A	30	19.122	28.372	8.654	1.00	249.25
70	1744	С	ASN A	30	19.863	24.172	8.412	1.00	244.43

	1745	0	ASN A	20	* 10.050	00.770			
	1748	Ñ	PHE A	30 31	19.859 20.478	23.770 23.527	7.252	1.00	244.43
	1747	CA	PHE A	31	21.210	23.327 22.326	9.386 9.077	1.00	249.41
_	1748	CB	PHE A	31	22.639	22.474	9.586	1.00 1.00	249.41
5	1749	CG	PHE A	31	23.362	23.675	9.073	1.00	249.46
	1750	CD1	PHE A	31	23.138	24.925	9.634	1.00	249.46 249.46
	1751	CD2	PHE A	31	24.250	23.563	8.008	1.00	249.46
	1752	CE1	PHE A	31	23.798	26.050	9.152	1.00	249.46
10	1753 1754	CE2	PHE A	31	24.917	24.682	7.514	1.00	249.46
10	1755	CZ C	PHE A PHE A	31	24.682	25.931	8.083	1.00	249.46
	1756	ŏ	PHE A	31 31	20.559 20. 22 6	21.049	9.617	1.00	249.41
	1757	Ň	PHE A	32	20.226	20.949 20.077	10.807 8.715	1.00	249.41
	1758	CA	PHE A	32	19.790	18.777	9.021	1.00 1.00	249.47
15	1759	CB	PHE A	32	18.496	18.614	8.228	1.00	249.47 246.45
	1760	CG	PHE A	32	17.642	17.487	8.707	1.00	246.45
	1761	CD1	PHE A	32	17.048	17.548	9.963	1.00	246.45
	1762	CD2	PHE A	32	17.442	16.359	7.921	1.00	246.45
20	1763 1764	CE1 CE2	PHE A	32	16.272	16.499	10.437	1.00	246.45
20	1765	CZ	PHE A PHE A	32 32	16.665	15.302	8.387	1.00	248.45
	1766	Č	PHE A	32	16.077 20.742	15.378 17.630	9.652	1.00	246.45
	1767	ŏ	PHE A	32	21.773	17.852	8.674 8.051	1.00	249.47
	1768	Ň	GLU A	33	20.392	16.403	9.058	1.00 1.00	249.47
25	1769	CA	GLU A	33	21.260	15.270	8.763	1.00	249.57 249.57
	1770	CB	GLU A	33	21.850	14.696	10.034	1.00	249.41
	1771	CG	GLU A	33	22.893	13.655	9.727	1.00	249.41
	1772 1773	CD OE1	GLU A	33	24.096	14.255	9.017	1.00	249.41
30	1774	OE2	GLU A GLU A	33	24.471	15.388	9.373	1.00	249.41
-	1775	C	GLU A	33 33	24.695 20.671	13.581 14.104	8.140	1.00	249.41
	1776	ŏ	GLU A	33	21.232	13.684	7.992 6.982	1.00 1.00	249.57
	1777	N	VAL A	34	19.566	13.554	8.485	1.00	249.57 216.78
25	1778	CA	VAL A	34	18.961	12.405	7.832	1.00	216.78
35	1779	CB	VAL A	34	17.623	12.017	8.499	1.00	196.07
	1780 1781	CG1	VAL A	34	17.008	10.816	7.801	1.00	196.07
	1782	CG2 C	VAL A VAL A	34	17.864	11.683	9.958	1.00	196.07
	1783	ŏ	VAL A VAL A	34 34	18.754 18.550	12.609	6.338	1.00	216.78
40	1784	Ň	SER A	35	18.845	13.729 11.506	5.860 5.608	1.00	216.78
	1785	CA	SER A	35	18.669	11.506	4.170	1.00 1.00	172.95 172.95
	1786	CB	SER A	35	19.837	10.789	3.489	1.00	249.26
	1787	og	SER A	35	19.822	9.399	3.775	1.00	249.26
45	1788 1789	C	SER A	35	17.368	10.770	3.873	1.00	172.95
73	1790	0 N	SER A SER A	35	16.978	10.632	2.715	1.00	172.95
	1791	CA	SER A	36 36	16.706 15.437	10.290 9.579	4.926	1.00	142.42
	1792	CB	SER A	36	15.404	9.579 8.320	4.773 5.643	1.00 1.00	142.42
	1793	OG	SER A	36	15.320	8.643	7.020	1.00	183.21 183,21
50	1794	C	SER A	20	14.288	10.498	5.168	1.00	142.42
	1795	0	SER A	36	13.906	10.585	6.337	1.00	142.42
	1796 1797	N CA	THR A	37	13.749	11.189	4.171	1.00	91.48
	1798	CB	THR A	37	12.645	12.117	4.370	1.00	91.48
55	1799	OG1	THR A THR A	37 37	13.088	13.579	4.085	1.00	110.07
	1800	CG2	THR A	37	14.193 11.960	13.929 14.535	4.928	1.00	110.07
	1801	c	THR A	37	11.582	11.689	4.352 3.366	1.00	110.07
	1802	0	THR A	37	11.902	11.294	2.244	1.00 1.00	91.48 91.48
60	1803	N	LYS A	38	10.321	11.748	3.769	1.00	121.21
60	1804	CA	LYS A	38	9.233	11.345	2.886	1.00	121.21
	1805 1806	CB	LYS A	38	8.339	10.344	3.600	1.00	152.68
	1807	CD	LYS A	38	9.088	9.131	4.112	1.00	152.68
	1808	CE	LYS A LYS A	38 38	8.151	8.168	4.824	1.00	152.68
65	1809	NZ	LYS A	38	8.877 7.952	6.909 5.951	5.245	1.00	152.68
	1810	C	LYS A	38	8.389	12.529	5.893 2.442	1.00 1.00	152.68
	1811	0	LYS A	38	8.140	13.440	3.226	1.00	121.21 121.21
	1812	N	TRP A	39	7.954	12.517	1.185	1.00	102.82
70	1813 1814	CA CB	TRP A	39	7.119	13.592	0.656	1.00	102.82
	1017	V B	TRP A	39	7.861	14.401	-0.401	1.00	80.70

	4040	00	TOO A	20	9.037	15.167	0.113	1.00	80.70
	1815	CG	TRP A	39					
	1816	CD2	TRP A	39	9.022	16.295	0.994	1.00	80.70
	1817	CE2	TRP A	39	10.366	16.677	1.201	1.00	80.70
	1818	CE3 .	TRP A	39	8.002	17.015	1.634	1.00	80.70
5		CD1	TRP A	39	10.351	14.922	-0.168	1.00	80.70
J	1819				11.154	15.826	0.484	1.00	80.70
	1820	NE1	TRP A	39					
	1821	CZ2	TRP A	39	10.717	17.745	2.011	1.00	80.70
	1822	CZ3	TRP A	39	8.355	18.082	2.443	1.00	80.70
	1823	CH2	TRP A	39	9.703	18.438	2.623	1.00	80.70
10					5.875	13.008	0.026	1.00	102.82
10	1824	Ç		39					
	1825	0	TRP A	39	5.956	12.079	-0.765	1.00	102.82
	1826	N	PHE A	40	4.724	13.562	0.368	1.00	102.87
	1827	CA	PHE A	40	3.489	13.049	-0.175	1.00	102.87
		CB	PHE A	40	2.633	12.434	0.936	1.00	104.88
	1828						1.706	1.00	
15	1829	CG	PHE A	40	3.319	11.346			104.88
	1830	CD1	PHE A	40	4.222	11.655	2.715	1.00	104.88
	1831	CD2	PHE A	40	3.050	10.011	1.438	1.00	104.88
	1832	CE1	PHE A	40	4.847	10.652	3.448	1.00	104.88
						8.999	2.167	1.00	104.88
	1833	CE2	PHE A	40	3.672				
20	1834	CZ	PHE A	40	4.570	9.321	3.174	1.00	104.88
	1835	С	PHE A	40	2.676	14.104	-0.898	1.00	102.87
	1836	Ö	PHE A	40	1.808	14.741	-0.302	1.00	102.87
				41	2.952	14.287	-2.184	1.00	73.61
	1837	N							
	1838	CA	HIS A	41	2.205	15.252	-2.984	1.00	73.61
25	1839	CB	HIS A	41	2.986	15.552	-4.254	1.00	81.93
	1840	CG	HIS A	41	2.304	16.514	-5.162	1.00	81.93
		CD2	HIS A	41	2.173	16.521	-6.507	1.00	81.93
	1841						-4.706	1.00	81.93
	1842	ND1	HIS A	41	1.661	17.645			
	1843	CE1	HIS A	41	1.158	18.309	-5.731	1.00	81.93
30	1844	NE2	HIS A	41	1.455	1 7.64 8	-6.837	1.00	81.93
-	1845	C	HIS A	41	0.811	14.687	-3.318	1.00	73.61
				41	0.690	13.733	-4.088	1.00	73.61
	1846	0						1.00	
	1847	N	ASN A	42	-0.234	15.280	-2.740		96.75
	1848	CA	ASN A	42	-1.617	14.822	-2.940	1.00	96.75
35	1849	CB	ASN A	42	-2.017	14.809	-4.435	1.00	98.09
55		ÇĞ	ASN A	42	-2.244	16.205	-5.004	1.00	98.09
	1850			42	-1.466	17.108	-4.726	1.00	98.09
	1851	OD1	ASN A						
	1852	ND2	ASN A	42	-3.284	16.385	-5.814	1.00	98.09
	1853	С	ASN A	42	<i>-</i> 1.771	13.413	-2.374	1.00	96.75
40	1854	0	ASN A	42	-2.625	12.652	-2.826	1.00	9 6.75
70		Ň	GLY A	43	-0.948	13.068	-1.386	1.00	89.87
	1855					11.739	-0.789	1.00	89.87
	1856	CA	GLY A	43	-1.019				
	1857	С	GLY A	43	-0.054	10.730	-1.410	1.00	89.87
	1858	0	GLY A	43	0.542	9.901	-0.714	1.00	89.87
45	1859	N	SER A	44	0.097	10.798	-2.728	1.00	129.29
,,,	1860	ĊA	SER A	44	0.990	9.904	-3.449	1.00	129.29
					0.833	10.113	-4.960	1.00	173.89
	1861	СВ	SER A	44					
	1862	OG	SER · A	44	-0.521	10.004	-5.358	1.00	173.89
	1863	С	SER A	44	2.436	10.182	-3.043	1.00	129.29
50	1864	0	SER A	44	2,890	11.322	-3.095	1.00	129.29
50		N	LEU A	45	3.159	9.142	-2.639	1.00	128.43
	1865					9.291	-2.239	1.00	128.43
	1866	CA	LEU A	45	4.559	9.291			
	1867	CB	LEU A	45	5.149	7.925	-1.874	1.00	210.08
	1868	CG	LEU A	45	6.602	7.911	-1.397	1.00	210.08
55	1869	CD1	LEU A	45	6.768	8.881	-0.237	1.00	210.08
25		CD2	LEU A	45	6.995	6.495	-0.980	1.00	210.08
	1870					9.921	-3.365	1.00	128.43
	1871	Ç	LEU A	45	5.379				
	1872	0	LEU A	45	5.129	9.671	-4.540	1.00	128.43
	1873	N	SER A	46	6.354	10.749	-3.007	1.00	150.05
60	1874	CA	SER A	46	7.200	11.403	-4.006	1.00	150.05
50	1875	CB	SER A	46	7.500	12.846	-3.588	1.00	129.32
								1.00	129.32
	1876	og.	SER A	46	8.251	13.516	-4.586		
	1877	C	SER A	46	8.499	10.623	-4.127	1.00	150.05
	1878	0	SER A	46	8.801	9.796	-3.275	1.00	150.05
65	1879	N	GLU A	47	9.274	10.881	-5.177	1.00	207.01
			GLU A	47	10.534	10.168	-5.357	1.00	207.01
	1880	CA							
	1881	CB	GLU A	47	10.798	9.896	-6.851	1.00	249.57
	1882	CG	GLU A	47	9.574	9.479	-7.672	1.00	249.57
	1883	CD	GLU A	47	9.801	9.602	-9.185	1.00	249.57
70	1884	OE1	GLU A	47	9.668	10.722	-9.729	1.00	249.57
70	, 504			•••	,				

	1885	OE2	GLU A	47	10.133	8.577	-9.821	1.00	249.57
	1886	č	GLU A	47	11.743	10.894	-4.739	1.00	207.01
	1887.	ŏ	GLU A	47	12.856	10.373	-4.796	1.00	207.01
_	1888	N	GLU A	48	11.556	12.084	-4.163	1.00	127.05
5	1889	CA	GLU A	48	12.703	12.760	-3.542	1.00	127.05
	1890	CB	GLU A	48	12.524	14.292 15.057	-3.489 -2.682	1.00 1.00	182.29
	1891	CG CD	GLU A GLU A	48 48	13.615 15.017	15.011	-3.296	1.00	182.29 182.29
	1892 1893	OE1	GLU A	48	15.226	15.631	-4.359	1.00	182.29
10	1894	OE2	GLU A	48	15.914	14.360	-2.713	1.00	182.29
	1895	C	GLU A	48	12.882	12.208	-2.126	1.00	127.05
	1896	0	GLU A	48	11.938	11.681	-1.531	1.00	127.05
	1897	N	THR A	49	14.099	12.305	-1.600	1.00	86.20
15	1898	CA	THR A	49 49	14.385 15.263	11.817 10.549	-0.258 -0.313	1.00 1.00	86.20 133.36
15	1899 1900	CB OG1	THR A THR A	49	16.473	10.832	-1.027	1.00	133.36
	1900	CG2	THR A	49	14.513	9.419	-1.021	1.00	133.36
	1902	C	THR A	49	15.074	12.903	0.583	1.00	86.20
	1903	0	THR A	49	14.950	12 938	1.810	1.00	86.20
20	1904	N ·	ASN A	50	15.787	13.801	-0.085	1.00	156.26
	1905	CA	ASN A	50	16.465	14.888	0.610 -0.406	1.00 1.00	156.26 185.93
	1906	CB CG +	ASN A ASN A	50 50	17.158 18.159	15.810 16.752	0.245	1.00	185.93
	1907 1908	OD1	ASN A	50	18.105	16.970	1.452	1.00	185.93
25	1909	ND2	ASN A	50	19.062	17.323	-0.549	1.00	185.93
	1910	C	ASN A	50	15.393	15.656	1.382	1.00	156.26
	1911	0	ASN A	50	14.238	15.689	0.976	1.00	156.26
	1912	N	SER A	51	15.765	16.264	2.499	1.00	124.65
30	1913	CA	SER A	51 51	14.804	17.019 17. 44 0	3.296 4.628	1.00 1.00	124.65 124.86
30	1914 1915	CB OG	SER A SER A	51 51	15.434 16.427	18.441	4.450	1.00	124.86
	1916	C	SER A	51	14.281	18.263	2.569	1.00	124.65
	1917	ŏ	SER A	51	13.257	18.823	2.959	1.00	124.65
	1918	N	SER A	52	14.979	18.704	1.525	1.00	90.69
35	1919	CA	SER A	52	14.553	19.884	0.780	1.00	90.69
	1920	CB	SER A	52	15.708	20.872	0.631 1.894	1.00 1.00	131.83 131.83
	1921 1922	OG C	SER A SER A	52 52	16.109 14.038	21.377 19.478	-0.584	1.00	90.69
	1923	ŏ	SER A	52	14.803	19.073	-1.449	1.00	90.69
40	1924	Ň	LEU A	53	12.727	19.584	-0.756	1.00	92.73
•	1925	CA	LEU A	53	12.057	19.239	-2.005	1.00	92.73
	1926	CB	LEU A	53	10.720	18.547	-1.710	1.00	96.57
	1927	CG	LEU A	53	9.633	18.561	-2.788	1.00	96.57 96.57
45	1928	CD1 CD2	LEU A LEU A	53 53	10.226 8.536	18.224 17.571	-4.145 -2,396	1.00 1.00	96.57
45	1929 1930	C	LEU A	53	11.814	20.486	-2.847	1.00	92.73
	1931	ŏ	LEU A	53	10.874	21.231	-2.601	1.00	92.73
	1932	N	ASN A	54	12.660	20.710	-3.846	1.00	74.24
	1933	CA	ASN A	54	12.508	21.879	-4.708	1.00	74.24
50	1934	CB	ASN A	54	13.819	22.180	-5.442	1.00	143.36
	1935	CG	ASN A ASN A	54 54	14.883 14.670	22.734 23.738	-4.526 -3.853	1.00 1.00	143.36 143.36
	1936 1937	OD1 ND2	ASN A	54	16.040	22.086	-4.497	1.00	143.36
	1938	C	ASN A	54	11.390	21.731	-5.727	1.00	74.24
55	1939	0	ASN A	54	10.937	20.633	-6.038	1.00	74.24
	1940	N	iLE A	55	10.936	22.868	-6.233	1.00	93.23
	1941	CA	ILE A	55	9.898	22.911	-7.249	1.00	93.23 75.25
	1942	CB CG2	ILE A ILE A	55 55	8.542 7.629	23.323 23.783	-6.659 -7.751	1.00 1.00	75.25 75.25
60	1943 1944	CG1	ILE A	55 55	7.932	22.135	-5.918	1.00	75.25
00	1945	CD1	ILE A	55	6.605	22.397	-5.286	1.00	75.25
	1946	C C	ILE A	55	10.359	23.951	-8.241	1.00	93.23
	1947	0	ILE A	55	10.593	25.100	-7.866	1.00	93.23
CF	1948	N	VAL A	56	10.528	23.543	-9.491	1.00	114.64
65	1949	CA CB	VAL A	56 56	10.977 12.025	24.469 23.820	-10.515 -11.410	1.00 1.00	114.64 202.78
	1950 1951	CB CG1	VAL A VAL A	56 56	12.025	24.892	-11.419 -12.183	1.00	202.78
	1952	CG2	VAL A	56	12.983	22.997	-10.579	1.00	202.78
	1953	C	VAL A	56	9.771	24.909	-11.333	1.00	114.64
70	1954	0	VAL A	56	8.649	24.730	-10.883	1.00	114.64

			A CN1 A	·	9.993	25.480	-12.516	1.00	86.89
	1955	N	ASN A ASN A	57 57	8.902	25.961	-13.366	1.00	86.89
	1956	CA	ASN A	57	9,187	25.646	-14.832	1.00	171.09
	1957	CB CG	ASN A	57	10.333	26.468	-15.379	1.00	171.09
5	1958	OD1	ASN A	57	10.332	27.695	-15.277	1.00	171.09
3	1959	ND2	ASN A	57	11.318	25.799	-15.962	1.00	171.09
	1960 1961	C	ASN A	57	7.549	25.397	-12.962	1.00	86.89
	1962	ŏ	ASN A	57	7.112	24.377	-13.473	1.00	86.89
	1963	N	ALA A	58	6.893	26.087	-12.036	1.00	98.74
10	1964	ĊA	ALA A	58	5.610	25.665	-11.500	1.00	98.74
10	1965	СВ	ALA A	58	5.094	26.705	-10.525	1.00	108.16
	1966	C	ALA A	58	4.557	25.376	-12.548	1.00	98.74
	1967	ō *	ALA A	58	4.185	26.242	-13.327	1.00	98.74
	1968	N	LYS A	59	4.082	24.140	-12.560	1.00	74.98
15	1969	CA	LYS A	59	3.039	23.725	-13.482	1.00	74.98
	1970	CB	LYS A	59	3.424	22.395	-14,146	1.00	178.83
	1971	CG	LYS A	59	4.740	22.455	-14.920	1.00	178.83
	1972	CD	LYS A	59	5.158	21.095	-15.463	1.00	178.83
	1973	CE	LYS A	59	6.483	21.185	-16.215	1.00 1.00	178.83 178.83
20	1974	NZ	LYS A	59	6.932	19.856 23.569	-16.725 -12.623	1.00	74.98
	1975	Ç	LYS A	59	1.782	23.163	-11.463	1.00	74.98
	1976	0	LYS A	59	1.878 0.614	23.912	-13.166	1.00	60.66
	1977	N	PHE A PHE A	60 60	-0.640	23.780	-12.418	1.00	60.66
25	1978	CA	PHE A	. 60	-1.815	23.834	-13.371	1.00	124.29
25	1979	CB CG	PHE A	60	-1.949	25.140	-14.046	1.00	124.29
	1980	CD1	PHE A	60	-2.524	25.234	-15.301	1.00	124.29
	1981 1982	CD2	PHE A	60	-1.510	26.294	-13.425	1.00	124.29
	1983	CE1	PHE A	60	-2.653	26.464	-15.942	1.00	124.29
30	1984	CE2	PHE A	60	-1.630	27.527	-14.054	1.00	124.29
50	1985	CZ	PHE A	60	-2.209	27.613	-15.313	1.00	124.29
	1986	C	PHE A	60	-0.714	22.496	-11.595	1.00	60.66
	1987	Ó	PHE A	60	-1.287	22.487	-10.504	1.00	60.66
	1988	N	GLU A	61	-0.124	21.418	-12.112	1.00	94.84
35	1989	CA	GLU A	61	-0.129	20.123	-11.433	1.00	94.84
	1990	СВ	GLU A	61	0.502	19.037	-12.312	1.00	214.43 214.43
	1991	CG	GLU A	61	-0.208	18.784	-13.625 -14.508	1.00 1.00	214.43
	1992	CD	GLU A	61	-0.246	20.011	-14.781	1.00	214.43
40	1993	OE1	GLU A	61	0.831	20.583 20.403	-14.930	1.00	214.43
40	1994	OE2	GLU A	61	-1.352 0.626	20.165	-10.114	1.00	94.84
	1995	C	GLU A GLU A	61 61	0.397	19.318	-9.253	1.00	94.84
	1996	0 N	ASP A	62	1.535	21.130	-9.959	1.00	76.23
	1997 1998	CA	ASP A	62	2.303	21.242	-8.728	1.00	76.23
45	1999	CB	ASP A	62	3.493	22,175	-8.913	1.00	161.53
73	2000	ca	ASP A	62	4.380	21.755	-10.072	1.00	161.53
	2001	OD1	ASP A	62	4.571	20.536	-10.273	1.00	161.53
	2002	OD2	ASP A	62	4.897	22.644	-10.778	1.00	161.53
	2003	C	ASP A	62	1.407	21.732	-7.614	1.00	76.23
50	2004	Ö	ASP A	62	1.721	21.544	-6.451	1.00	76.23
	2005	N	SER A	63	0.280	22,341	-7.977	1.00	83.22
	2006	CA	SER A	63	-0.680	22.828	-6.992	1.00	83.22
	2007	CB	SER A	63	-1.880	23.464	-7.691	1.00	115.03
	2008	OG	SER A	63	-1.503	24.633	-8.399	1.00	115.03 83.22
55	2009	Ç	SER A	63	-1.140	21.621	-6.212	1.00 1.00	83.22
	2010	0	SER A	63	-1.508	20.640	-6.814 -4.887	1.00	65.94
	2011	N.	GLY A	64	-1.124	21.660	-4.154	1.00	65.94
	2012	CA	GLY A	64	-1.575	20.488 20.493	-2.661	1.00	65.94
60	2013	C	GLY A	64	-1.306	21.530	-2.082	1.00	65.94
60	2014	0	GLY A	64 65	-0.942 -1.509	19.337	-2.032	1.00	82.22
	2015	N	GLU A GLU A	65 65	-1.285	19.159	-0.605	1.00	82.22
	2016	CA	GLU A	65	-2.463	18.376	-0.031	1.00	143.82
	2017 2018	CB CG	GLU A	65	-2.304	17.897	1.394	1.00	143.82
65	2018	CD	GLU A	65	-3.356	16.866	1.773	1.00	143.82
UJ	2019	OE1	GLU A	65	-3.374	15.779	1.157	1.00	143.82
	2020	OE2	GLU A	65	-4.169	17.139	2.681	1.00	143.82
	2022	c	GLU A	65	0.035	18.378	-0.420	1.00	82.22
	2023	ŏ	GLU A	65	0.207	17.313	-1.011	1.00	82.22
70	2024	N	TYR A	66	0.971	18.903	0.374	1.00	76.24

		C4	TVD A	cc .	2.240	18.224	0.614	1.00	76.24
	2025	CA	TYR A	66		19.083	0.150	1.00	67.69
	2026	CB	TYR A	66	3.377	19.339	-1.314	1.00	67.69
	2027	CG .	TYR A	66	3.426	20.255	-1.915	1.00	67.69
_	2028	CD1	TYR A	66	2.574	20.572	-3.265	1.00	
5	2029	CE1	TYR A	66	2.680		-2.095	1.00	67.69
	2030	CD2	TYR A	66	4.385	18.724	-3.447	1.00	67.69
	2031	CE2	TYR A	66	4.502	19.017	-4.032	1.00	67.69
	2032	CZ	TYR A	66	3.647	19.948	-5.378	1.00	67.69
	2033	ОH	TYR A	66	3.792	20.230			67.69
10	2034	Č	TYR A	66	2.490	17.934	2.083	1.00	76.24
	2035	0	TYR A	66	1.891	18.570	2.941	1.00	76.24
	2036	N	LYS A	67	3.398	17.000	2.375	1.00	93.48
	2037	CA	LYS A	67	3.756	16.664	3.759	1.00	93.48
	2038	CB	LYS A	67	2.619	15.924	4.439	1.00	143.97
15	2039	CG	LYS A	67	2.079	14.788	3.619	1.00	143.97
	2040	CD	LYS A	67	0.876	14.176	4.291	1.00	143.97
	2041	CE	LYS A	67	0.213	13.163	3.385	1.00	143.97
	2042	NZ	LYS A	67	-1.009	12.616	4.023	1.00	143.97
	2043	С	LYS A	67	5.011	15.818	3.806	1.00	93.48
20	2044	0	LYS A	67	5.357	15.166	2.824	1.00	93.48
	2045	N	CYS A	68	5.715	15.852	4.932	1.00	71.26
	2046	CA	CYS A	68	6.914	15.044	5.067	1.00	71.26
	2047	C	CYS A	68	6.823	14.232 '	6.340	1.00	71.26
	2048	0	CYS A	68	6.020	14.540	7.208	1.00	71.26
25	2049	CB	CYS A	68	8.183	15.905	5.041	1.00	93.73
	2050	SG	CYS A	68	8.385	17.184	6.305	1.00	93.73
	2051	N	GLN A	69	7.619	13.174	6.425	1.00	106.93
	2052	CA	GLN A	69	7.651	12.302	7.591	1.00	106.93
	2053	СВ	GLN A	69	6.558	11. 23 3	7.476	1.00	95.79
30	2054	CG	GLN A	69	6.744	10.032	8.390	1.00	95.79
	2055	CD	GLN A	69	5.702	8.954	8.161	1.00	95.79
	2056	OE1	GLN A	69	5.476	8.521	7.024	1.00	95.79
	2057	NE2	GLN A	69	5.060	8.509	9.244	1.00	95.79
	2058	С	GLN A	69	9.015	11.641	7.629	1.00	106.93
35	2059	0	GLN A	69	9.657	11.496	6.594	1.00	106.93
	2060	N	HIS A	70	9.462	11.243	8.813	1.00	174.41
	2061	CA	HIS A	70	10.753	10.589	8.928	1.00	174.41
	2062	CB	HIS A	70	11.601	11.296	9.977	1.00	160 <i>.2</i> 7
	2063	CG	HIS A	70	12.022	12.673	9.572	1.00	160. 2 7
40	2064	CD2	HIS A	70	11.502	13.885	9.873	1.00	160 <i>.2</i> 7
	2065	ND1	HIS A	70	13.085	12.909	8.726	1.00	160.27
	2066	CE1	HIS A	70	13.203	14.210	8.527	1.00	160 <i>.2</i> 7
	2067	NE2	HIS A	70	12.257	14.824	9.213	1.00	160. 2 7
	2068	C	HIS A	70	10.632	9.112	9.268	1.00	. 174.41
45	2069	Ö	HIS A	70	9.543	8.536	9.237	1.00	174.41
	2070	N	GLN A	71	11.764	8.505	9.590	1.00	242.81
	2071	CA	GLN A	71	11.815	7.091	9.923	1.00	242.81
	2072	СВ	GLN A	71	13.246	6.724	10.335	1.00	199.62
	2073	CG	GLN A	71	13.632	5.293	9.992	1.00	199.62
50	2074	CD	GLN A	71	13.345	4.945	8.543	1.00	199.62
	2075	OE1	GLN A	71	14.015	5.423	7.634	1.00	199.62
	2076	NE2	GLN A	71	12.331	4.115	8.324	1.00	199.62
	2077	C	GLN A	71	10.817	6.722	11.027	1.00	242.81
	2078	Ö	GLN A	71	9.989	5.829	10.844	1.00	242.81
55	2079	Ň	GLN A	72	10.886	7.419	12.160	1.00	160.50
	2080	CA	GLN A	72	9.991	7.143	13.289	1.00	160.50
	2081	CB	GLN A	72	10.803	6.584	14.465	1.00	249.38
	2082	ÇĞ	GLN A	72	9.972	6.150	15.671	1.00	249.38
	2083	ÇD	GLN A	72	10.819	5.563	16.791	1.00	249.38
60	2084	OE1	GLN A	72	11.537	4.581	16.594	1.00	249.38
v	2085	NE2	GLN A	72	10.738	6.164	17.975	1.00	249.38
	2086	Ċ	GLN A	72	9.237	8.392	13.740	1.00	160.50
	2087	ŏ	GLN A	72	9.319	8. 79 7	14.901	1.00	160.50
	2088	Ň	VAL A	73	8.493	9.001	12.825	1.00	139.31
65	2089	ČA	VAL A	73	7.759	10.217	13.154	1.00	139.31
33	2090	CB	VAL A	73	8.575	11.467	12.795	1.00	182.81
	2091	CG1	VAL A	73	7.960	12.688	13.430	1.00	182.81
	2092	CG2	VAL A	73	10.000	11.297	13.237	1.00	182.81
	2092	C	VAL A	73	6.445	10.284	12.391	1.00	139,31
70	2094	ŏ	VAL A	73	6.352	9.819	11.254	1.00	139.31
, 0	200	_							

				•			40.040	4.00	00.24
	2095	N	ASN A	74	5.428	10.864	13.019	1.00	98.24
	2096	CA	ASN A	74	4.136	10.988	12.376	1.00	98.24
	2097	СВ	ASN A	74	3.045	11.209	13.427	1.00	227.24
	2098	ČĠ	ASN A	74	3.039	10.124	14.489	1.00	227.24
5	2099	OD1	ASN A	74	3.176	8.940	14.170	1.00	227.24
5		ND2	ASN A	74	2.875	10.520	15.748	1.00	227.24
	2100		ASN A	74	4.194	12.144	11.378	1.00	98.24
	2101	C		74	4.649	13.246	11.700	1.00	98.24
	2102	0	ASN A		3.750	11.863	10.157	1.00	124.76
	2103	Ņ	GLU A	75		12.842	9.074	1.00	124.76
10	2104	CA	GLU A	75	3.730	12.302	7,921	1.00	249.33
	2105	CB	GLU A	75	2.881		8.364	1.00	249.33
	2106	CG	GLU A	75	1.709	11.440			
	2107	CD	GLU A	75	1.032	10.734	7.202	1.00	249.33
	2108	OE1	GLU A	7 5	1.730	10.023	6.446	1.00	249.33
15	2109	OE2	GLU A	75	-0.198	10.888	7.048	1.00	249.33
15	2110	C	GLU A	75	3.245	14.232	9.499	1.00	124.76
	2111	ŏ	GLU A	75	2.346	14.372	10.327	1.00	124.76
		Ň	SER A	76	3.859	15.255	8.912	1.00	84.02
	2112	· CA	SER A	76	3.569	16.653	9.208	1.00	84.02
20	2113		SER A	76	4.578	17.534	8.509	1.00	92.60
20	2114	CB		76	4.391	17.395	7.108	1.00	92.60
	2115	og	SER A		2.201	17.096	8.754	1.00	84.02
	2116	Ç	SER A	76		16.468	7.888	1.00	84,02
	2117	0	SER A	76	1.599		9.323	1.00	82.56
	2118	N	GLU A	77	1.722	18.198			82.56
25	2119	CA	GLU A	77	0.415	18.751	8.960	1.00	211.53
	2120	CB	GLU A	77	೮.ಮಿರ	19.918	9.883	1.00	
	2121	CG	GLU A	77	-0.157	19.511	11.331	1.00	211.53
	2122	CD	GLU A	77	-1.343	18.579	11.512	1.00	211.53
	2123	OE1	GLU A	77	-1.831	18.020	10. 50 5	1.00	211.53
30		OE2	GLU A	77	-1.780	18.396	12.668	1.00	211.53
20	2124	C	GLU A	77	0.550	19.239	7.533	1.00	82.56
	2125		GLU A	77	1.397	20.102	7.252	1.00	82.56
	2126	0		78	-0.250	18.679	6.604	1.00	57.51
	2127	N	PRO A		-1.105	17.493	6.808	1.00	210.77
	2128	CD	PRO A	78 70	-0.226	19.047	5,186	1.00	57.51
35	2129	CA	PRO A	78		18.370	4.644	1.00	210.77
	2130	CB	PRO A	78	-1.469		5.376	1.00	210.77
	2131	CG	PRO A	78	-1.440	17.076	4.936	1.00	57.51
	2132	C	PRO A	78	-0.193	20.544	5.785	1.00	57.51
	2133	0	PRO A	78	-0.607	21.338		1.00	75.93
40	2134	N	VAL A	79	0.343	20.931	3.789		75.93
	2135	CA	VAL A	79	0.396	22.331	3.422	1.00	
	2136	СВ	VAL A	79	1.780	22.859	3.574	1.00	49.48
	2137	CG1	VAL A	79	1.916	24.215	2.850	1.00	49.48
	2138	CG2	VAL A	79	2.078	23.010	5.039	1.00	49.48
45	2139	Č	VAL A	79	-0.033	22.466	1.972	1.00	75.93
43		ŏ	VAL A	79	0.463	21.748	1.113	1.00	75.93
	2140		TYR A	80	-0.961	23.375	1.696	1.00	60.67
	2141	N		80	-1.424	23.519	0.336	1.00	60.67
	2142	CA		80	2.903	23.814	0.280	1.00	249.12
	2143	CB	TYR A		-3.420	23.538	-1.115	1.00	249.12
50	2144	CG	TYR A.	80		22.256	-1.623	1.00	249.12
	2145	CD1	TYR A	80	-3.434	22.005	-2.920	1.00	249.12
	2146	CE1	TYR A	80	-3.870			1.00	249.12
	2147	CD2	TYR A	80	-3.902	24.575	-1.927	1.00	249.12
	2148	CE2	TYR A	80	-4.414	24.332	-3.216	1.00	
55	2149	CZ	TYR A	80	-4.378	23.015	-3.703	1.00	249.12
75	2150	OH	TYR A	80	-4.926	22.722	-4.929	1.00	249.12
	2151	C	TYR A	80	-0.736	24.582	-0.438	1.00	20.67
	2152	ŏ	TYR A	80	-0.537	25.688	0.043	1.00	60.67
		Ň	LEU A	81	-0.414	24.264	-1 .66 9	1.00	53.62
60	2153		LEU A	81	0.237	25.227	-2.520	1.00	53.62
60		CA			1.547	24.619	-3.003	1.00	66.18
	2155	CB	LEU A	81	2.237	25.486	-4.035	1.00	66.18
	2156	CG	LEU A	81			-3.373	1.00	66.18
	2157	CD1	LEU A	81	2.603	26.806		1.00	66.18
	2158	CD2	LEU A	81	3.461	24.803	-4.566 2.600	1.00	53.62
65	2159	С	LEU A	81	-0.703	25.487	-3.698		53.62
	2160	0	LEU A	81	-1.229	24.534	-4.283	1.00	
	2161	Ň	GLU A	82	-0.956	26.742	-4.048	1.00	63.15
	2162	CA	GLU A	82	-1.821	26.990	-5.201	1.00	63.15
	2163	CB	GLU A	82	-3.099	27.700	-4.772	1.00	149.46
70	2164	cg	GLU A	82.	-4.259	27.463	-5.722	1.00	149.46
70	, 2104	•		 .					

2185										
2166 OE1 GLU A 82 -5.788 22.194 -4.050 1.00 1.00 1.00 1.00 1.00 1.00 1.00		0165	CD	GLUA	82	-5.537	28.157	-5.276	1.00	149.46
2167 OE2 GLU A 82 -6.286 24.653 -6.151 1.00								-4.050	1.00	149.46
2168 C GLU A 82 -1.100 27.823 -5.996 1.00 2170 N VAL A 83 -1.157 27.352 -7.525 1.00 2171 CA VAL A 83 -1.157 27.352 -7.525 1.00 2171 CB VAL A 83 0.194 27.803 -8.516 1.00 2173 CG1 VAL A 83 0.194 27.803 -8.516 1.00 2174 CG2 VAL A 83 0.194 27.803 -8.516 1.00 2175 C VAL A 83 1.294 28.427 -8.739 1.00 2176 O VAL A 83 1.294 28.427 -8.739 1.00 2177 N PHE A 84 1.473 28.859 -9.501 1.00 2177 N PHE A 84 -1.942 30.088 -8.539 1.00 2177 N PHE A 84 -1.942 30.088 -8.539 1.00 2178 CA PHE A 84 -1.947 30.947 -10.632 1.00 2180 CA PHE A 84 -1.947 30.947 -7.488 1.00 2181 CD1 PHE A 84 -1.945 31.304 -7.488 1.00 2181 CD1 PHE A 84 -4.503 11.074 -7.488 1.00 2183 CE1 PHE A 84 -4.503 11.09 11.764 -7.324 1.00 2184 CD2 PHE A 84 -4.521 31.312 -6.242 1.00 2185 CD2 PHE A 84 -1.947 30.941 -9.248 1.00 2186 CC PHE A 84 -1.943 31.09 11.080 -6.323 1.00 2187 C PHE A 84 -1.943 31.09 11.09 11.09 11.09 11.00										149.46
21770			C	GLU A						63.15
2177 CA VAL A 83 -0.517 28.050 -8.632 1.00 2178 CO2 VAL A 83 0.749 27.819 -10.728 1.00 2178 CO2 VAL A 83 0.749 27.819 -10.728 1.00 2178 CO2 VAL A 83 1.244 28.447 -8.738 1.00 2176 C VAL A 83 1.473 28.559 -9.501 1.00 2177 C VAL A 83 1.473 28.559 -9.501 1.00 2176 C VAL A 83 1.473 28.559 -9.501 1.00 2177 N PHE A 84 1.082 30.088 -9.839 1.00 2178 CA PHE A 84 1.082 30.088 -9.839 1.00 2179 CB PHE A 84 1.0947 30.047 10.632 1.00 2180 CG PHE A 84 2.395 32.164 -9.834 1.00 2180 CG PHE A 84 2.345 31.300 31.836 -8.588 1.00 2181 CD1 PHE A 84 3.130 31.836 -8.588 1.00 2182 CD2 PHE A 84 3.130 31.306 -8.588 1.00 2183 CE1 PHE A 84 3.134 31.108 -6.323 1.00 2185 CZ PHE A 84 4.521 31.312 -6.242 1.00 2186 CZ PHE A 84 4.521 31.312 -6.242 1.00 2186 CZ PHE A 84 4.519 31.764 -7.324 1.00 2187 O PHE A 84 1.390 31.480 11.323 1.00 2188 N SER A 85 2.237 31.895 12.717 1.00 2189 CA SER A 85 2.237 31.895 12.717 1.00 2190 CB SER A 85 2.237 31.895 1.2771 1.00 2191 OG SER A 85 2.237 31.895 1.00.717 1.00 2192 C SER A 85 2.2999 33.835 11.3599 1.00 2193 O SER A 85 2.245 33.774 1.5142 1.00 2194 N ASPA 86 3.209 38.256 1.38.89 1.00 2196 CB ASPA 86 3.209 38.256 1.38.89 1.00 2197 CG ASPA 86 3.209 38.256 1.38.89 1.00 2198 OD ASPA 86 6.5443 38.277 1.2599 1.00 2200 C ASPA 86 6.5443 38.277 1.3344 1.00 2201 O ASPA 86 6.5443 38.277 1.3344 1.00 2202 N TRP A 87 -2.688 41.090 1.00 2203 CA TRP A 87 -2.688 41.090 1.14.007 1.00 2204 CB TRP A 87 -1.803 38.867 1.3349 1.00 2205 CG TRP A 87 -1.803 38.867 1.3249 1.00 2206 CD TRP A 87 -1.803 38.867 1.3249 1.00 2207 TRP A 87 -1.803 38.867 1.3249 1.00 2208 CG TRP A 87 -1.803 38.867 1.3249 1.00 2209 C TRP A 87 -1.803 38.867 1.3249 1.00 2200 C ASPA 86 -5.425 33.670 1.44.007 1.00 2201 O ASPA 86 -5.426 33.670 1.44.007 1.00 2202 N TRP A 87 -2.688 41.090 1.44.857 1.00 2203 CA TRP A 87 -1.803 38.867 1.3249 1.00 2204 CB TRP A 87 -1.803 38.867 1.3249 1.00 2205 CG TRP A 87 -1.803 40.088 1.2249 1.00 2206 CD TRP A 87 -1.803 40.088 1.2249 1.00 2216 CB CB LEU A 88 -2.245 33.670 1.3349 1.00 2217 CG LEU A 88 -2.245 33.670 1.4049 1.0049 1.00 22	5	2169								63.15 58.52
21772 CGB VAL A 83 0.164 27.085 -9.516 1.00 2173 CG2 VAL A 83 1.294 28.427 -9.738 1.00 2174 CG2 VAL A 83 1.294 28.427 -9.738 1.00 2175 C VAL A 83 1.294 28.427 -9.738 1.00 2176 C VAL A 83 1.294 28.427 -9.738 1.00 2177 C VAL A 83 1.294 28.427 -9.738 1.00 2177 C VAL A 83 1.294 28.427 -9.738 1.00 2178 C VAL A 83 1.294 28.427 -9.738 1.00 2177 C VAL A 83 1.294 28.427 -9.738 1.00 2177 C VAL A 83 1.294 28.427 -9.738 1.00 2177 C VAL A 83 1.294 28.427 -9.738 1.00 2177 C VAL A 83 1.294 28.429 -9.677 1.00 2178 C A PHE A 84 1.947 30.947 -10.632 1.00 2180 C B PHE A 84 3.130 31.836 -9.588 1.00 2181 C C B PHE A 84 3.130 31.836 -9.588 1.00 2182 C D PHE A 84 4.503 32.031 8.498 1.00 2183 C D PHE A 84 4.503 32.031 8.498 1.00 2184 C C PHE A 84 5.199 31.764 -7.324 1.00 2185 C PHE A 84 1.380 31.480 11.923 1.00 2186 C PHE A 84 1.380 31.482 12.179 1.00 2187 C PHE A 84 1.380 31.482 12.179 1.00 2188 C PHE A 84 0.186 31.482 12.179 1.00 2189 C B SER A 85 2.297 31.985 12.717 1.00 2180 C B SER A 85 2.297 31.985 12.717 1.00 2190 C B SER A 85 2.297 31.985 12.717 1.00 2191 C G SER A 85 2.299 33.835 11.399 1.00 30 2194 N ASP A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 85 2.299 33.835 11.399 1.00 31 2194 C B SER A 85 2.299 33.835 11.399 1.00 31 2194 C B SER A 86 2.299 33.835 11.399 1.00 31 2194 C B SER A 86 2.296 35.033 11.386 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 32 2195 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2194 C B SER A 86 3.299 33.835 11.399 1.00 31 2195 C B SER A 86 3.299 33.835 11.399 1.00 31 2196 C B SER A 86 3.299 33.835 11.399 1.00 31 2197 C B SER A 86 3.299 33.835 11.399 1.00 31 2198 C B SER A 86 3.299 33.835										58.52
1173										61.79
10 2174										61.79
2176 C VAL A 83 -1.473 28.859 -9.501 1.00 2176 O VAL A 83 -2.540 28.364 -9.877 1.00 2177 N PHE A 84 -1.082 30.088 -9.839 1.00 2178 CA PHE A 84 -1.082 30.088 -9.839 1.00 2178 CB PHE A 84 -1.092 30.088 -9.839 1.00 2179 CB PHE A 84 -1.092 30.088 -9.839 1.00 2180 CG PHE A 84 -2.395 32.164 -9.834 1.00 2180 CG PHE A 84 -2.395 32.164 -9.834 1.00 2181 CD1 PHE A 84 -2.455 31.374 -7.488 1.00 2181 CD2 PHE A 84 -4.503 32.031 -8.488 1.00 2182 CD2 PHE A 84 -4.503 32.031 -8.488 1.00 2183 CE1 PHE A 84 -4.503 32.031 -8.488 1.00 2184 CE2 PHE A 84 -4.503 32.031 -8.488 1.00 2185 CZ PHE A 84 -4.503 31.374 -7.324 1.00 2186 C PHE A 84 -4.521 31.312 -6.242 1.00 2187 C PHE A 84 -4.521 31.312 -6.242 1.00 2188 N SER A 85 -2.237 31.985 12.179 1.00 2189 CA SER A 85 -2.267 32.625 -13.989 1.00 2190 C SER A 85 -2.214 32.358 -15.378 1.00 2191 OG SER A 85 -2.214 32.358 -15.378 1.00 2191 OG SER A 85 -2.214 32.358 -15.378 1.00 2192 C SER A 85 -2.2453 31.714 -15.142 1.00 2193 O SER A 85 -2.2453 31.714 -15.142 1.00 2194 C SER A 85 -2.2463 33.670 -14.007 1.00 30 2194 N ASP A 86 -3.209 32.556 -13.803 1.00 2195 CA ASP A 86 -3.209 32.556 -13.803 1.00 2196 CB ASP A 86 -3.209 32.556 -13.803 1.00 2197 CG ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803 1.00 2198 CB ASP A 86 -3.209 32.556 -13.803	10								1.00	61.79
2176 O VAL A 83 -2.540 28.384 -9.877 1.00 2177 N PHE A 84 -1.002 30.088 -9.839 1.00 2180 CA PHE A 84 -1.947 30.947 10.652 1.00 2181 CD1 PHE A 84 -2.395 32.164 -9.834 1.00 2181 CD1 PHE A 84 -2.395 32.164 -9.834 1.00 2181 CD1 PHE A 84 -2.455 31.374 -7.488 1.00 2182 CD2 PHE A 84 -4.503 32.031 -8.489 1.00 2183 CE1 PHE A 84 -4.503 32.031 -8.489 1.00 2184 CE2 PHE A 84 -4.503 32.031 -8.489 1.00 2185 CZ PHE A 84 -4.521 31.310 31.836 -6.323 1.00 2186 C PHE A 84 -4.521 31.312 -6.242 1.00 2187 C PHE A 84 -4.521 31.312 -6.242 1.00 2188 N SER A 84 -1.390 31.480 11.923 1.00 2189 CA SER A 85 -2.067 32.625 13.989 1.00 2180 CA SER A 85 -2.067 32.625 13.989 1.00 2181 CD3 SER A 85 -2.453 31.714 15.142 1.00 2182 C SER A 85 -2.453 31.714 15.142 1.00 2183 O SER A 85 -2.453 31.714 15.142 1.00 2184 N ASP A 86 -2.453 33.670 11.959 1.00 30 2194 N ASP A 86 -3.209 33.635 11.3599 1.00 2196 CB ASP A 86 -3.209 33.635 11.3599 1.00 2197 CG ASP A 86 -4.226 33.670 14.007 1.00 31 2190 CB ASP A 86 -5.454 33.625 13.803 1.00 2194 N ASP A 86 -5.454 33.625 13.803 1.00 2195 CA ASP A 86 -5.454 33.625 13.803 1.00 2196 CB ASP A 86 -5.454 33.625 13.803 1.00 2197 CG ASP A 86 -5.00 36.296 12.599 1.00 2198 CD1 ASP A 86 -5.454 33.927 12.599 1.00 2200 C ASP A 86 -5.433 33.037 14.007 1.00 2201 O ASP A 86 -5.433 33.037 14.007 1.00 2202 N TIPP A 87 -2.760 38.661 14.004 1.00 2203 CA TIPP A 87 -2.632 41.339 1.5914 1.00 2204 CB TIPP A 87 -2.632 41.339 1.5914 1.00 2205 CG TIPP A 87 -3.996 40.723 15.915 1.00 2206 CD2 TIPP A 87 -3.996 40.723 15.915 1.00 2207 CE2 TIPP A 87 -3.996 40.723 15.915 1.00 2208 CE3 TIPP A 87 -4.834 40.509 1.9261 1.00 2207 CE TIPP A 87 -3.996 40.499 1.2448 1.000 1.00 2208 CE3 TIPP A 87 -5.608 39.231 1.9389 1.00 2209 CB TIPP A 87 -5.608 39.231 1.9389 1.00 2200 C ASP A 86 -5.009 39.231 1.9386 1.00 2201 N TIPP A 87 -5.608 39.231 1.9386 1.00 2202 C TIPP A 87 -5.608 39.231 1.9386 1.00 2203 CA TIPP A 87 -5.608 39.231 1.9386 1.00 2204 CB TIPP A 87 -5.608 39.231 1.9386 1.00 2216 CB TIPP A 87 -5.608 39.231 1.9386 1.00 2217 CG LEU A 88 -0.404 41.399 38.470	10									58.52
2177 N PHE A 84 -1.092 30.098 9.8.93 1.00 2178 CA PHE A 84 -1.947 30.0947 10.6522 1.00 2180 CG PHE A 84 -2.395 32.164 9.834 1.00 2181 CD1 PHE A 84 -2.395 32.164 9.834 1.00 2182 CD2 PHE A 84 -2.455 31.374 7.488 1.00 2183 CE1 PHE A 84 -4.503 32.031 -8.498 1.00 2184 CE2 PHE A 84 -4.503 32.031 -8.498 1.00 2185 CZ PHE A 84 -4.503 32.031 -8.498 1.00 2186 C PHE A 84 -5.199 31.764 -7.324 1.00 2186 C PHE A 84 -5.199 31.764 -7.324 1.00 2186 C PHE A 84 -5.199 31.764 -7.324 1.00 2186 C PHE A 84 -1.309 31.480 11.923 1.00 2187 O PHE A 84 -1.309 31.480 11.923 1.00 2188 N SER A 85 -2.327 31.985 12.717 1.00 2189 CA SER A 85 -2.327 31.985 12.717 1.00 2190 CB SER A 85 -2.2453 31.714 15.142 1.00 2191 OG SER A 85 -2.453 31.714 15.142 1.00 2192 C SER A 85 -2.214 32.335 11.395 1.00 2193 O SER A 85 -2.299 33.835 113.959 1.00 2194 N ASP A 86 -3.209 36.256 13.835 10.00 2195 CA ASP A 86 -3.209 36.256 13.803 1.00 2196 CB ASP A 86 -4.131 30.259 1.2589 1.00 2197 CG ASP A 86 -5.433 30.097 13.3455 1.00 2198 OD1 ASP A 86 -5.433 30.097 13.3455 1.00 2199 OD2 ASP A 86 -5.433 30.097 13.3455 1.00 2200 C ASP A 86 -5.433 30.097 13.3455 1.00 2201 O ASP A 86 -5.433 30.097 13.3455 1.00 2202 C ASP A 86 -5.433 30.097 13.3455 1.00 2203 CA TRP A 87 -2.260 38.661 14.004 1.00 2204 CB TRP A 87 -2.268 41.090 1.44.57 1.00 2205 CD TRP A 87 -2.268 41.090 1.44.57 1.00 2206 CD TRP A 87 -3.596 40.723 1.6830 1.00 2207 CP TRP A 87 -3.596 40.723 1.6830 1.00 2208 CB TRP A 87 -2.268 41.090 1.44.57 1.00 2208 CB TRP A 87 -3.596 40.723 1.6830 1.00 2209 CD TRP A 87 -3.596 40.723 1.6830 1.00 2201 C ASP A 86 -2.245 37.453 1.3756 1.00 2202 CD TRP A 87 -3.596 40.723 1.9584 1.00 2203 CA TRP A 87 -3.596 40.723 1.9584 1.00 2204 CB TRP A 87 -3.596 40.723 1.9584 1.00 2205 CD TRP A 87 -3.596 40.723 1.9584 1.00 2206 CD TRP A 87 -3.596 40.723 1.9584 1.00 2207 CE2 TRP A 87 -3.596 40.723 1.9584 1.00 2208 CB 3 TRP A 87 -2.268 41.090 1.44.57 1.00 2209 CD TRP A 87 -3.590 40.499 1.9831 1.00 2216 C EEU A 88 -1.497 4.399 38.470 1.0333 1.00 2221 C C EEU A 88 -1.497 4.399 38.470 1.004 2222 C C EEU					83					58.52
15 2179 CB PHE A 84 2.395 32.164 9.834 1.00 2180 CG PHE A 84 -2.455 31.374 -7.488 1.00 2181 CD1 PHE A 84 -2.455 31.374 -7.488 1.00 2182 CD2 PHE A 84 -2.455 31.374 -7.488 1.00 2183 CE1 PHE A 84 -3.134 31.108 -8.233 1.00 2183 CE1 PHE A 84 -3.134 31.108 -8.233 1.00 2185 CZ PHE A 84 -4.519 31.764 -7.324 1.00 2185 CZ PHE A 84 -4.521 31.312 -6.242 1.00 2186 C PHE A 84 -4.521 31.312 -6.242 1.00 2186 C PHE A 84 -1.390 31.486 11.1223 1.00 2187 O PHE A 84 -1.390 31.486 11.1223 1.00 2187 O PHE A 84 -1.390 31.486 11.1223 1.00 2188 CA SER A 85 -2.327 31.885 -12.717 1.00 2188 CA SER A 85 -2.327 31.885 -12.717 1.00 2189 CB SER A 85 -2.2667 32.625 13.989 1.00 2191 OG SER A 85 -2.214 32.588 -16.378 1.00 2191 OG SER A 85 -2.214 32.588 -16.378 1.00 2191 OG SER A 85 -2.299 33.835 -13.399 1.00 2191 OG SER A 85 -2.299 33.835 -13.399 1.00 2191 OG SER A 85 -2.299 33.835 -13.399 1.00 2192 C SER A 85 -2.299 33.835 -13.399 1.00 2192 C SER A 85 -2.293 33.835 -13.399 1.00 2192 C SER A 85 -2.294 33.670 -14.007 1.00 2192 C C SER A 85 -2.299 33.835 -13.399 1.00 2193 C C ASP A 86 -3.209 33.835 -13.399 1.00 2198 CB ASP A 86 -3.209 33.835 -13.399 1.00 2198 CB ASP A 86 -3.209 33.835 -13.399 1.00 2198 CB ASP A 86 -5.453 31.714 -15.142 1.00 2198 CB ASP A 86 -5.454 33.6027 -12.876 1.00 2198 CB ASP A 86 -5.454 33.8087 -13.345 1.00 2198 CB ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.8087 -13.345 1.00 2202 C ASP A 86 -5.454 33.80										70.51 70.51
19										69.94
2181 CD1 PHE A 84 - 2.455 31.374 - 7.488 1.00 2182 CD2 PHE A 84 - 3.134 31.08	12									69.94
2182 CD2 PHE A 84 4.503 32.031 8.488 1.00 2183 CE1 PHE A 84 3.134 31.08 6.323 1.00 2184 CE2 PHE A 84 5.199 31.764 -7.324 1.00 2186 C PHE A 84 4.521 31.312 6.222 1.00 2187 C PHE A 84 4.521 31.312 6.222 1.00 2188 N SER A 84 4.521 31.312 6.222 1.00 2188 N SER A 85 2.2327 31.885 1.2.717 1.00 2189 CA SER A 85 2.2067 32.625 13.989 1.00 2190 CB SER A 85 2.2453 31.714 15.142 1.00 2191 OG SER A 85 2.2453 31.714 15.142 1.00 2191 OG SER A 85 2.2453 31.714 15.142 1.00 2192 C SER A 85 2.2599 33.835 1.3.959 1.00 2193 O SER A 85 2.299 33.835 1.3.959 1.00 2194 N ASP A 86 3.209 33.835 1.3.959 1.00 2195 CA ASP A 86 2.425 35.033 13.803 1.00 2196 CB ASP A 86 3.209 38.256 13.805 1.00 2197 CG ASP A 86 4.131 38.259 1.2599 1.00 310 2198 OD1 ASP A 86 5.454 38.0827 12.876 1.00 32199 OD2 ASP A 86 5.454 38.0827 12.876 1.00 32199 OD2 ASP A 86 6.509 38.626 12.629 1.00 32199 OD2 ASP A 86 6.509 38.626 12.629 1.00 32200 C ASP A 86 6.509 38.626 12.629 1.00 3201 C ASP A 86 7.265 37.453 13.756 1.00 2202 N TRP A 87 2.260 38.661 14.004 1.00 2203 CA TRP A 87 2.668 41.033 39.848 14.009 1.00 2204 CB TRP A 87 2.668 41.033 39.848 14.000 1.00 2205 CG TRP A 87 3.596 40.723 16.683 1.00 2206 CD2 TRP A 87 3.596 40.723 16.683 1.00 2207 CE2 TRP A 87 3.596 40.723 16.683 1.00 2208 CE3 TRP A 87 -2.668 41.033 39.848 14.000 1.00 2209 CE3 TRP A 87 -3.596 40.723 16.683 1.00 2211 CZ2 TRP A 87 -3.596 40.723 16.683 1.00 2211 CZ2 TRP A 87 -3.596 40.723 16.683 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.820 1.00 2212 CD LEU A 88 -2.496 44.139 -9.857 1.00 2213 CH2 TRP A 87 -5.528 39.887 -17.820 1.00 2214 CB LEU A 88 -2.496 44.139 -9.857 1.00 2215 CD LEU A 88 -2.496 44.139 -9.857 1.00 2226 CB LEU A 88 -2.496 44.193 -9.857 1.00 2227 CG LEU A 88 -2.495 33.342 -5.177 1.00 2222 CD LEU A 89 -0.425 33.342 -5.177 1.00										69.94
2183 CE1 PHE A 84 3.134 31.108 -6.323 1.00 2185 CZ PHE A 84 -5.199 31.764 -7.324 1.00 2185 CZ PHE A 84 -5.199 31.764 -7.324 1.00 2185 CZ PHE A 84 -5.193 31.764 -7.324 1.00 2187 O PHE A 84 -1.390 31.480 1.11.923 1.00 2187 O PHE A 84 -1.390 31.480 1.11.923 1.00 2187 O PHE A 84 -1.390 31.480 1.11.923 1.00 2188 N SER A 85 -2.327 31.985 1.2717 1.00 2188 N SER A 85 -2.327 31.985 1.2717 1.00 2191 OG SER A 85 -2.453 31.714 15.142 1.00 2191 OG SER A 85 -2.243 31.714 15.142 1.00 2191 OG SER A 85 -2.243 31.714 15.142 1.00 2191 OG SER A 85 -2.2999 33.835 115.578 1.00 2192 C SER A 85 -2.2999 33.835 115.578 1.00 2193 O SER A 85 -4.226 33.670 14.007 1.00 30 2194 N ASP A 86 -2.245 35.033 11.3836 1.00 2196 CB ASP A 86 -3.209 36.256 13.836 1.00 2196 CB ASP A 86 -3.209 36.256 13.836 1.00 2198 CB ASP A 86 -5.454 36.827 12.879 1.00 2198 OD1 ASP A 86 -5.454 36.827 12.879 1.00 2200 C ASP A 86 -5.454 38.827 12.879 1.00 2200 C ASP A 86 -5.454 38.827 12.879 1.00 2200 C ASP A 86 -5.454 38.827 12.879 1.00 2200 C ASP A 86 -6.509 38.256 11.3.00 1.00 2200 C ASP A 86 -6.245 37.453 13.356 1.00 2200 C ASP A 86 -6.245 37.453 13.356 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2200 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 2201 C ASP A 86 -1.043 37.284 13.502 1.00 22									1.00	69.94
20 2184 CE2 PHE A 84 -5.199 31.764 -7.324 1.00 2185 CZ PHE A 84 -4.521 31.312 -6.242 1.00 2186 C PHE A 84 -1.390 31.480 11.923 1.00 2187 O PHE A 84 -1.390 31.480 11.923 1.00 2187 O PHE A 84 -0.186 31.452 12.1719 1.00 2188 N SER A 85 -2.327 31.985 12.717 1.00 2190 CB SER A 85 -2.067 32.625 13.895 1.00 2190 CB SER A 85 -2.453 31.714 15.142 1.00 2190 CB SER A 85 -2.453 31.714 15.142 1.00 2190 CB SER A 85 -2.453 31.714 15.142 1.00 2190 CB SER A 85 -2.214 32.359 16.378 1.00 2190 C SER A 85 -2.299 33.835 13.959 1.00 2190 C SER A 85 -2.299 33.835 13.959 1.00 2190 C SER A 85 -2.299 33.835 13.959 1.00 2190 C SER A 85 -2.299 33.835 13.959 1.00 2190 C A ASP A 86 -2.425 35.03 13.836 1.00 2195 CA ASP A 86 -2.425 35.03 13.836 1.00 2196 CB ASP A 86 -2.425 35.03 13.836 1.00 2197 C3 ASP A 86 -3.209 36.256 13.803 11.00 2197 C3 ASP A 86 -4.131 36.259 12.599 1.00 2199 CD ASP A 86 -5.454 36.927 12.876 1.00 2200 C ASP A 86 -5.454 36.927 12.876 1.00 2200 C ASP A 86 -5.454 36.927 12.876 1.00 2200 C ASP A 86 -5.454 37.453 13.756 1.00 2200 C ASP A 86 -2.245 37.453 39.807 13.345 1.00 2200 C							31.108			69.94
2185 CZ PHE A 84 4.521 31.312 -0.242 1.00 2186 C PHE A 84 -1.390 31.480 11.923 1.00 2187 O PHE A 84 -0.186 31.452 12.179 1.00 2188 N SER A 85 -2.2067 32.625 13.889 1.00 2198 CA SER A 85 -2.2067 32.625 13.889 1.00 2190 CB SER A 85 -2.2067 32.625 13.889 1.00 2191 OG SER A 85 -2.2067 32.625 13.889 1.00 2191 OG SER A 85 -2.214 32.358 16.378 1.00 2192 C SER A 85 -2.214 32.358 16.378 1.00 2193 O SER A 85 -2.214 32.358 16.378 1.00 2194 N ASP A 85 -2.214 32.358 16.378 1.00 2195 CA SER A 85 -2.214 32.358 16.378 1.00 2196 CB ASP A 86 -2.245 35.033 1.3836 1.00 2196 CB ASP A 86 -3.209 93.255 13.836 1.00 2196 CB ASP A 86 -3.209 36.256 13.803 1.00 2198 OD1 ASP A 86 -5.433 38.057 13.345 1.00 2198 OD1 ASP A 86 -5.433 38.057 13.356 1.00 2198 OD2 ASP A 86 -6.609 38.256 12.629 1.00 2200 C ASP A 86 -6.2245 37.453 13.756 1.00 2201 O ASP A 86 -2.245 37.453 13.756 1.00 2202 N TRP A 87 -2.760 38.661 14.004 1.00 2203 CA TRP A 87 -2.608 41.000 1.00 2204 CB TRP A 87 -2.608 41.000 1.00 2205 CG TRP A 87 -2.608 41.000 1.00 2206 CG TRP A 87 -3.506 40.723 -16.830 1.00 2207 CE2 TRP A 87 -3.506 40.723 -16.830 1.00 2208 CD1 TRP A 87 -2.608 41.000 1.8122 1.00 2209 CD1 TRP A 87 -2.608 41.000 1.8122 1.00 2201 NEI TRP A 87 -3.506 40.723 -16.830 1.00 2202 TRP A 87 -3.506 40.723 -16.830 1.00 2203 CA TRP A 87 -3.506 40.723 -16.830 1.00 2204 CB TRP A 87 -3.500 39.923 -19.68 1.00 2205 CG TRP A 87 -3.500 39.923 -19.265 1.00 2206 CG TRP A 87 -3.500 40.086 -1.6.633 1.00 2207 CE2 TRP A 87 -3.500 40.086 -1.6.633 1.00 2208 CD1 TRP A 87 -4.668 41.000 -1.8122 1.00 2209 CD1 TRP A 87 -4.668 41.000 -1.8122 1.00 2210 NEI TRP A 87 -5.008 39.923 -19.285 1.00 2211 CD2 LEU A 88 -2.496 44.139 -9.837 1.00 2212 CD3 TRP A 87 -5.008 39.923 -19.285 1.00 2213 CH2 LEU A 88 -2.496 44.139 -9.837 1.00 2224 C LEU A 88 -2.496 44.139 -9.837 1.00 2226 CB LEU A 89 -1.466 33.878 -9.899 1.00 2226 CB LEU A 89 -1.466 33.800 -5.784 1.00 2226 CB LEU A 89 -1.466 33.800 -5.784 1.00 2226 CB LEU A 89 -1.466	20		CE2							69.94
2187 O PHE A 84 -0.196 31.452 .12.179 1.00 2188 N SER A 85 -2.327 31.985 .12.717 1.00 2189 CA SER A 85 -2.267 32.625 .13.989 1.00 2190 CB SER A 85 -2.463 31.714 .15.142 1.00 2191 OG SER A 85 -2.267 32.625 .13.989 1.00 2191 OG SER A 85 -2.267 32.625 .13.989 1.00 2192 C SER A 85 -2.299 33.835 .13.578 1.00 2193 O SER A 85 -2.299 33.835 .13.559 1.00 2194 N ASP A 86 -2.245 33.670 .14.007 1.00 2195 CA ASP A 86 -2.245 33.670 .14.007 1.00 2196 CB ASP A 86 -3.209 36.256 .13.803 1.00 2197 CG ASP A 86 -4.131 39.259 .12.589 1.00 2198 OD1 ASP A 86 -5.433 38.087 .13.345 1.00 2198 OD1 ASP A 86 -5.433 38.087 .13.345 1.00 2200 C ASP A 86 -6.509 36.256 .13.803 1.00 2201 O ASP A 86 -1.269 36.256 .13.803 1.00 2202 N TRP A 87 -2.760 38.661 14.004 1.00 2202 N TRP A 87 -2.7668 41.090 .10.04 1.00 2203 CA TRP A 87 -2.632 41.233 .15.756 1.00 2204 CB TRP A 87 -2.632 41.233 .15.754 1.00 2205 CG TRP A 87 -2.668 41.090 .14.591 1.00 2206 CG TRP A 87 -2.668 41.090 .14.591 1.00 2207 CE2 TRP A 87 -2.668 41.090 .14.591 1.00 2208 CE3 TRP A 87 -2.668 41.090 .14.591 1.00 2207 CE2 TRP A 87 -3.506 40.723 .16.830 1.00 2219 CC3 TRP A 87 -1.618 41.757 .16.663 1.00 2210 NE1 TRP A 87 -1.618 41.757 .16.663 1.00 2211 CC2 TRP A 87 -1.618 41.757 .16.663 1.00 2212 CC3 TRP A 87 -1.618 41.757 .16.663 1.00 2214 C TRP A 87 -1.618 41.757 .16.663 1.00 2216 NE1 TRP A 87 -1.618 41.757 .16.663 1.00 2217 CA LEU A 88 -2.496 44.139 .9.837 .100 2218 CG LEU A 88 -2.496 44.139 .9.837 .100 2216 CG LEU A 88 -2.496 44.139 .9.837 .100 2217 CA LEU A 88 -2.496 44.139 .9.837 .100 2226 CG LEU A 88 -2.496 44.139 .9.837 .100 2226 CG LEU A 88 -2.496 44.139 .9.837 .100 2226 CG LEU A 88 -2.496 44.139 .9.837 .100 2216 CD LEU A 88 -2.305 33.944 .100 .100 2227 CG LEU A 88 -2.496 44.139 .9.837 .100 2226 CG LEU A 89 -1.768 33.944 .100 .100 2226 CG LEU A 89 -1.768 33.944 .100 .100 2226 CG LEU A 89 -1.768 33.944 .100 .100 2226 CG LEU A 89 -1.768 33.944 .100 .100 2226 CG LEU A 89 -1.456 33.973 .9.859 1.00 2227 CG LEU A 89 -1.456 33.973 .9.859 1.00 2226 CD LEU A 89 -1.456 33.930 .9.571 1.00 2226										69.94 70.51
2188 N SER A 85 -2.327 31.985 -12.717 1.00 2190 CB SER A 85 -2.067 32.625 -13.989 1.00 2191 OG SER A 85 -2.463 31.714 -15.142 1.00 2192 C SER A 85 -2.214 32.358 -16.378 1.00 2192 C SER A 85 -2.214 32.358 -16.378 1.00 2193 O SER A 85 -2.245 33.670 -14.007 1.00 30 2194 N ASP A 86 -2.425 33.670 -14.007 1.00 2195 CA ASP A 86 -3.209 36.256 -13.803 1.00 2196 CB ASP A 86 -3.209 36.256 -13.803 1.00 2197 CG ASP A 86 -5.433 38.087 -12.576 1.00 31 2198 OD1 ASP A 86 -5.433 38.087 -12.576 1.00 32 2199 OD2 ASP A 86 -5.433 38.087 -13.345 1.00 31 2199 OD2 ASP A 86 -6.509 36.296 -12.589 1.00 2200 C ASP A 86 -2.245 37.453 -13.756 1.00 2201 O ASP A 86 -1.043 37.284 -13.502 1.00 2202 N TRP A 87 -2.760 38.661 -14.004 1.00 2203 CA TRP A 87 -2.682 41.233 -15.914 1.00 2204 CB TRP A 87 -2.682 41.233 -15.914 1.00 2205 CG TRP A 87 -2.682 41.233 -15.914 1.00 2206 CG TRP A 87 -3.5100 40.950 -18.122 1.00 2207 CE2 TRP A 87 -3.3100 40.950 -18.122 1.00 2208 CE3 TRP A 87 -3.3100 40.950 -18.122 1.00 2210 CC TRP A 87 -3.3100 40.950 -18.122 1.00 2211 CZ2 TRP A 87 -3.3100 40.950 -18.122 1.00 2211 CZ2 TRP A 87 -3.3100 40.950 -18.122 1.00 2211 CZ2 TRP A 87 -3.3100 40.950 -18.122 1.00 2211 CZ2 TRP A 87 -3.3100 40.950 -18.122 1.00 2212 CZ3 TRP A 87 -5.528 39.887 -17.820 1.00 2213 CH2 TRP A 87 -1.891 41.586 -17.994 1.00 2214 C TRP A 87 -1.693 39.923 -19.086 1.00 2215 CA LEU A 88 -2.2457 41.681 -9.805 1.00 2216 N LEU A 88 -2.2457 41.681 -9.805 1.00 2221 CD LEU A 88 -2.2457 41.681 -9.805 1.00 2222 C LEU A 88 -2.2467 41.681 -9.805 1.00 2223 C LEU A 88 -1.863 40.372 -10.255 1.00 2224 C LEU A 88 -2.305 39.273 -9.359 1.00 2225 C LEU A 89 -1.456 38.978 -9.359 1.00 2226 CB LEU A 89 -1.456 38.978 -9.359 1.00 2227 CG LEU A 89 -1.459 39.008 -5.784 1.00 2226 CB LEU A 89 -1.459 39.008 -5.784 1.00 2227 CG LEU A 89 -1.459 39.008 -5.785 1.00 2228 CD1 LEU A 89 -0.429 39.008 -5.785 1.00 2226 CB LEU A 89 -0.429 39.008 -5.785 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2233 CA LEU A 90 -2.240 38.815 3.3760 1.00										70.51
25 2189 CA SER A 85 -2.067 32.625 -13.989 1.00 2190 CB SER A 85 -2.453 31.714 -15.142 1.00 2191 OG SER A 85 -2.214 32.358 -16.378 1.00 2192 C SER A 85 -2.214 32.358 -16.378 1.00 2192 C SER A 85 -2.214 32.358 -16.378 1.00 2193 O SER A 85 -2.214 32.358 -16.378 1.00 30 2194 N ASP A 86 -2.425 33.670 -14.007 1.00 30 2196 CB ASP A 86 -2.425 33.633 -13.836 1.00 2196 CB ASP A 86 -3.209 36.256 -13.803 1.00 2197 CG ASP A 86 -4.131 36.259 -12.599 1.00 2198 OD1 ASP A 86 -5.454 36.827 -12.876 1.00 2198 OD1 ASP A 86 -5.454 36.827 -12.876 1.00 2200 C ASP A 86 -6.509 36.256 -12.629 1.00 2201 O ASP A 86 -1.043 37.284 -13.756 1.00 2201 O ASP A 86 -1.043 37.284 -13.756 1.00 2202 N TRP A 87 -2.668 41.090 -14.457 1.00 2203 CA TRP A 87 -2.668 41.090 -14.457 1.00 2204 CB TRP A 87 -2.668 41.090 -14.457 1.00 2205 CG TRP A 87 -3.596 40.723 -15.914 1.00 2206 CD2 TRP A 87 -3.596 40.723 -15.914 1.00 2207 CE2 TRP A 87 -3.596 40.723 -15.914 1.00 2208 CE3 TRP A 87 -4.834 40.077 -16.686 1.00 2210 NE1 TRP A 87 -1.618 41.757 -16.666 1.00 2211 CZ2 TRP A 87 -5.528 39.887 -17.220 1.00 2212 CZ3 TRP A 87 -5.528 39.887 -17.220 1.00 2213 CH2 TRP A 87 -5.528 39.887 -17.220 1.00 2214 C TRP A 87 -1.618 41.757 -16.666 1.00 2216 N LEU A 88 -2.457 41.681 -9.805 1.00 2217 CA LEU A 88 -2.459 40.140 -11.673 1.00 2218 CB LEU A 88 -2.457 41.681 -9.805 1.00 2219 CG LEU A 88 -2.457 41.681 -9.805 1.00 2220 CB LEU A 88 -2.457 41.681 -9.805 1.00 2221 CD2 LEU A 88 -1.863 40.372 -0.023 1.00 2222 C LEU A 88 -2.457 41.681 -9.805 1.00 2226 CB LEU A 89 -1.456 38.973 -9.550 1.00 2227 CG LEU A 89 -1.456 38.973 -9.550 1.00 2226 CB LEU A 89 -1.456 38.973 -9.550 1.00 2227 CG LEU A 89 -1.456 38.973 -9.550 1.00 2221 CD2 LEU A 89 -1.459 38.470 -6.036 1.00 2221 CD2 LEU A 89 -1.459 38.470 -6.036 1.00 2223 C C LEU A 89 -1.459 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00										86.88
2190 CB SER A 85 -2.453 31.714 -15.142 1.00 2191 OG SER A 85 -2.245 32.358 -16.378 1.00 2192 C SER A 85 -2.219 33.835 -13.959 1.00 2193 O SER A 85 -2.299 33.835 -13.959 1.00 30 2194 N ASP A 86 -2.425 35.633 -13.836 1.00 2195 CA ASP A 86 -3.209 36.256 -13.803 1.00 2196 CB ASP A 86 -3.209 36.256 -13.803 1.00 2197 CG ASP A 86 -5.433 38.087 -12.599 1.00 316 2198 OD1 ASP A 86 -5.433 38.087 -12.599 1.00 32198 OD1 ASP A 86 -5.433 38.087 -12.599 1.00 317 CG ASP A 86 -5.433 38.087 -13.345 1.00 32200 C ASP A 86 -5.433 38.087 -13.345 1.00 2201 O ASP A 86 -5.433 38.087 -13.345 1.00 2202 N TRP A 86 -5.433 39.087 -13.356 1.00 2204 CB TRP A 87 -2.760 38.661 -14.004 1.00 2203 CA TRP A 87 -2.760 38.661 -14.004 1.00 2204 CB TRP A 87 -2.668 41.090 -14.457 1.00 2205 CG TRP A 87 -2.682 41.233 -15.914 1.00 2206 CG TRP A 87 -3.596 40.723 -16.683 1.00 2207 CE2 TRP A 87 -3.596 40.723 -16.683 1.00 2210 CE3 TRP A 87 -1.618 41.757 -16.666 1.00 2210 CE3 TRP A 87 -1.618 41.757 -16.663 1.00 2211 CT2 TRP A 87 -1.618 41.757 -16.663 1.00 2211 CT2 TRP A 87 -1.618 41.757 -16.663 1.00 2212 CT2 TRP A 87 -1.618 41.757 -16.663 1.00 2213 CH2 TRP A 87 -5.008 39.923 -19.986 1.00 2214 C TRP A 87 -5.008 39.923 -19.086 1.00 2216 N E1 TRP A 87 -1.618 41.757 -16.683 1.00 2217 CA LEU A 88 -2.249 40.140 -11.673 1.00 2218 CB LEU A 88 -2.249 40.140 -11.673 1.00 2219 CG LEU A 88 -2.249 40.140 -11.673 1.00 2210 CD LEU A 88 -2.249 40.140 -11.673 1.00 2221 CD LEU A 88 -2.805 39.274 -9.389 1.00 2222 C LEU A 88 -3.399 38.723 -9.551 1.00 2223 C LEU A 89 -1.456 38.979 39.008 -5.784 1.00 2226 CB LEU A 89 -1.459 39.235 -9.551 1.00 2227 CG LEU A 89 -1.459 39.235 -9.551 1.00 2228 CD LEU A 89 -1.459 39.008 -5.784 1.00 2226 CB LEU A 89 -1.459 39.008 -5.784 1.00 2227 CG LEU A 89 -1.459 39.008 -5.785 1.00 2228 CD LEU A 89 -1.459 39.008 -5.785 1.00 2226 CB LEU A 89 -1.459 39.008 -5.785 1.00 2227 CG LEU A 89 -1.459 39.008 -5.785 1.00 2228 CD LEU A 89 -1.459 39.008 -5.785 1.00 2221 CD LEU A 89 -1.459 39.008 -5.785 1.00 2223 CD LEU A 89 -0.429 39.008 -5.785 1.00 2233 CA LEU A 90 -2	25									86.88
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2192 C SER A 85 -2.999 33,835 -13,595 1.00 2194 N ASP A 86 -2.425 35,033 -13,836 1.00 2195 CA ASP A 86 -2.425 35,033 -13,836 1.00 2196 CB ASP A 86 -3,209 36,256 -13,803 1.00 2197 CG ASP A 86 -5,454 36,927 -12,599 1.00 2198 OD1 ASP A 86 -5,454 36,927 -12,599 1.00 2198 OD2 ASP A 86 -5,453 38,087 -13,345 1.00 2199 OD2 ASP A 86 -6,509 36,226 -12,629 1.00 2200 C ASP A 86 -6,509 36,226 -13,803 -13,345 1.00 2201 O ASP A 86 -1,404 37,224 -13,502 1.00 2201 O ASP A 86 -1,404 37,224 -13,502 1.00 2202 N TRP A 87 -2,760 38,661 -14,004 1.00 2203 CA TRP A 87 -2,668 41,090 -14,457 1.00 2204 CB TRP A 87 -2,668 41,090 -14,457 1.00 2206 CG TRP A 87 -3,3100 40,950 -18,122 1.00 2207 CE2 TRP A 87 -3,3100 40,950 -18,122 1.00 2208 CE3 TRP A 87 -4,834 40,077 -16,683 1.00 2211 CG2 TRP A 87 -1,891 41,586 -17,994 1.00 2211 CG2 TRP A 87 -1,891 41,586 -17,994 1.00 2211 CG2 TRP A 87 -1,891 41,586 -17,994 1.00 2211 CG2 TRP A 87 -1,891 41,586 -17,994 1.00 2211 CG2 TRP A 87 -1,891 41,586 -17,994 1.00 2211 CG2 TRP A 87 -3,794 40,549 -19,261 1.00 2211 CG2 TRP A 87 -3,794 40,549 -19,261 1.00 2212 CC3 TRP A 87 -5,508 39,923 -19,086 1.00 2213 CH2 TRP A 87 -5,508 39,923 -19,086 1.00 2216 N LEU A 88 -2,496 44,139 -12,468 1.00 2217 CA LEU A 88 -2,496 44,139 -9,837 1.00 2221 CC2 LEU A 88 -2,395 39,794 40,995 1.00 2217 CG LEU A 88 -2,395 39,794 -10,492 1.00 2218 CB LEU A 88 -2,496 44,139 -9,837 1.00 2221 CC2 LEU A 88 -1,907 42,914 -10,492 1.00 2217 CG LEU A 88 -2,496 44,139 -9,837 1.00 2226 CB LEU A 89 -1,769 37,943 -7,432 1.00 2227 CG LEU A 89 -1,769 37,943 -7,432 1.00 2228 CD1 LEU A 89 -1,769 37,943 -7,432 1.00 2226 CB LEU A 89 -1,769 37,943 -7,432 1.00 2227 CG LEU A 89 -1,769 37,943 -7,432 1.00 2228 CD1 LEU A 89 -1,459 38,470 -7,636 1.00 2230 C LEU A 89 -1,459 38,470 -7,636 1.00 2231 C LEU A 89 -0,425 38,345 -5,176 1.00 2232 CD LEU A 89 -0,425 38,345 -5,176 1.00 2233 C LEU A 89 -0,425 38,345 -5,176 1.00 2233 C LEU A 89 -0,425 38,345 -5,176 1.00 2233 C LEU A 89 -0,425 38,342 -5,177 1.00								-16.378		135.23
2193						-2.999				86.88
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2196 CB ASP A 86 -4.131 38.259 -12.589 1.00 2197 CG ASP A 86 -5.454 38.927 -12.876 1.00 2198 OD1 ASP A 86 -5.454 38.927 -12.876 1.00 35 2199 OD2 ASP A 86 -6.509 38.296 -12.629 1.00 2200 C ASP A 86 -6.509 38.296 -12.629 1.00 2201 O ASP A 86 -2.245 37.453 -13.756 1.00 2202 N TRP A 87 -2.760 38.661 -14.004 1.00 2203 CA TRP A 87 -2.760 38.661 -14.004 1.00 2204 CB TRP A 87 -2.682 41.090 -14.457 1.00 2205 CG TRP A 87 -2.682 41.090 -14.457 1.00 2206 CD2 TRP A 87 -3.596 40.723 -16.830 1.00 2207 CE2 TRP A 87 -3.596 40.723 -16.683 1.00 2208 CE3 TRP A 87 -3.5100 40.950 -18.122 1.00 2209 CD1 TRP A 87 -1.618 41.757 -16.666 1.00 2211 CZ2 TRP A 87 -1.891 41.586 -17.994 1.00 2211 CZ2 TRP A 87 -1.891 41.586 -17.994 1.00 2212 CZ3 TRP A 87 -5.508 39.923 -19.088 1.00 2213 CH2 TRP A 87 -5.008 39.923 -19.088 1.00 2216 N LEU A 88 -2.496 44.139 -9.857 1.00 2217 CA LEU A 88 -2.496 44.139 -9.857 1.00 2221 CD2 LEU A 88 -1.907 42.914 -10.492 1.00 2222 CB LEU A 89 -1.459 37.443 -7.452 1.00 2223 CD2 LEU A 89 -1.459 37.443 -7.452 1.00 2224 CB LEU A 89 -1.459 37.443 -7.452 1.00 2225 CB LEU A 89 -1.459 37.443 -7.452 1.00 2226 CB LEU A 89 -1.459 37.443 -7.452 1.00 2227 CG LEU A 89 -1.769 37.443 -7.452 1.00 2228 CD1 LEU A 89 -1.769 37.443 -7.452 1.00 2221 CD2 LEU A 89 -1.769 37.443 -7.452 1.00 2222 CB LEU A 89 -1.769 37.443 -7.452 1.00 2223 CD LEU A 89 -1.769 37.443 -7.452 1.00 2224 CD2 LEU A 89 -1.769 37.443 -7.452 1.00 2225 CA LEU A 89 -1.769 37.443 -7.452 1.00 2226 CB LEU A 89 -1.769 37.443 -7.452 1.00 2227 CG LEU A 89 -1.769 37.443 -7.452 1.00 2228 CD1 LEU A 89 -1.769 37.443 -7.452 1.00 2226 CB LEU A 89 -1.769 37.443 -7.452 1.00 2227 CG LEU A 89 -1.459 38.470 -7.066 1.00 2231 C LEU A 89 -1.459 38.470 -7.066 1.00 2231 C LEU A 89 -1.459 38.470 -7.066 1.00 2232 CD2 LEU A 89 -1.459 38.470 -7.066 1.00 2232 CD2 LEU A 89 -1.459 38.470 -7.066 1.00 2232 CD2 LEU A 89 -0.429 39.008 -5.784 1.00 2233 CA LEU A 90 -2.245 39.008 -5.784 1.00	30									47.41 47.41
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2218 CB LEU A 88 -2.457 41.681 -9.805 1.00 55 2219 CG LEU A 88 -1.907 42.914 -10.492 1.00 2220 CD1 LEU A 88 -2.496 44.139 -9.837 1.00 2221 CD2 LEU A 88 -0.394 42.908 -10.383 1.00 2222 C LEU A 88 -2.305 39.274 -9.369 1.00 2223 O LEU A 88 -3.399 38.723 -9.501 1.00 60 2224 N LEU A 89 -1.456 38.978 -8.399 1.00 2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -0.902 36.718 -7.675 1.00 2228 CD1 LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -0.455 34.401 -7.046 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2231 O LEU A 89 -0.455 34.401 -7.046 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 89 -0.429 39.008 -5.784 1.00 2233 CA LEU A 90 -2.459 38.342 -5.127 1.00				LEU A						74.08
55 2219				LEU A						74.08
2220 CD1 LEU A 88 -2.496 44.139 -9.837 1.00 2221 CD2 LEU A 88 -0.394 42.908 -10.383 1.00 2222 C LEU A 88 -2.305 39.274 -9.369 1.00 2223 O LEU A 88 -3.399 38.723 -9.501 1.00 2224 N LEU A 89 -1.456 38.978 -8.399 1.00 2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 2230 C LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -0.455 34.401 -7.046 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 89 -0.429 39.008 -5.784 1.00 2233 CA LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00				LEU A						87.26 87.26
2221 CD2 LEU A 88 -0.394 42.908 -10.383 1.00 2222 C LEU A 88 -2.305 39.274 -9.369 1.00 2223 O LEU A 88 -3.399 38.723 -9.501 1.00 2224 N LEU A 89 -1.456 38.978 -8.399 1.00 2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -1.769 37.943 -7.432 1.00 2227 CG LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 2228 CD1 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.240 38.815 -3.760 1.00	55			LEU A						87.26
2222 C LEU A 88 -2.305 39.274 -9.369 1.00 2223 O LEU A 88 -3.399 38.723 -9.501 1.00 60 2224 N LEU A 89 -1.456 38.978 -8.399 1.00 2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -1.769 37.943 -7.432 1.00 2227 CG LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.249 39.008 -5.784 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00									1.00	87.26
2223 O LEU A 88 -3.399 38.723 -9.501 1.00 60 2224 N LEU A 89 -1.456 38.978 -8.399 1.00 2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00										74.08
60 2224 N LEU A 89 -1.456 38.978 -8.399 1.00 2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -0.455 34.401 -7.046 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00										74.08
2225 CA LEU A 89 -1.769 37.943 -7.432 1.00 2226 CB LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00	60			LEU A						49.26
2226 C8 LEU A 89 -0.902 36.718 -7.675 1.00 2227 CG LEU A 89 -1.170 35.653 -6.637 1.00 2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00	00			LEU A						49.26
2228 CD1 LEU A 89 -2.692 35.436 -6.511 1.00 65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00				LEU A						70.28
65 2229 CD2 LEU A 89 -0.455 34.401 -7.046 1.00 2230 C LEU A 89 -1.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00								-6.63/ e.511		70.28 70.28
2230 C LEU A 891.499 38.470 -6.036 1.00 2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00	15									70.28
2231 O LEU A 89 -0.429 39.008 -5.784 1.00 2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00	60			LEU A						49.26
2232 N LEU A 90 -2.459 38.342 -5.127 1.00 2233 CA LEU A 90 -2.240 38.815 -3.760 1.00										49.26
2233 CA LEU A 90 -2.240 38.815 -3.760 1.00							38.342	-5.127		72.68
			CA	LEU A	90	-2.240				72.68
	70	2234	CB	LEU A	90	3.562	39.231	-3.111	1.00	33.75

	2235	CG	LEU A	90	-3.444	39.630	-1.648	1.00	33.75
	2236	CD1	LEU A	90	-2.488	40.814	-1.620	1.00	33.75
	2237	CD2	LEU A	90	-4.790	40.011	-1.047	1.00	33.75
_	2238	C	LEU A	90	-1.623 -2.254	37.701 36.674	-2.931 -2.710	1.00 1.00	72.68 72.68
5	2239 2240	O N	LEU A GLN A	90 91	-2.25 4 -0.398	37.896	-2.462	1.00	48.17
	2240	CA	GLN A	91	0.255	ଅମ.864	-1.656	1.00	48.17
	2242	СВ	GLN A	91	1.692	36,682	-2.110	1.00	50.84
	2243	CG	GLN A	91	1.773	36.315	-3.559	1.00	50.84
10	2244	CD	GLN A	91	3.159	35.954	-3.971	1.00	50.84
	2245	OE1	GLN A GLN A	91	4.041 3.371	36.801 34.688	-4.013 -4.271	1.00 1.00	50.84 50.84
	2246 2247	NE2 C	GLN A	91 91	0.218	37.151	-0 165	1.00	48.17
	2248	ŏ	GLN A	91	0.282	38.298	0. 254	1.00	48.17
15	2249	Ň	ALA A	92	0.098	36.113	0.648	1.00	56.37
	2250	CA	ALA A	92	0.044	36.326	80ن.2	1.00	56.37
	2251	CB	ALA A	92	-1.329	36.039	2.579	1.00	37.31 56.37
	2252	. C	ALA A ALA A	92 92	1.033 1. 2 02	35.422 24.266	2.769 2.381	1.00 1.00	56.37 56.37
20	2253 2254	N	SER A	93	1.695	35.939	3.794	1.00	55.78
20	2255	CA	SER A	93	2.665	35.146	4.535	1.00	55.78
	2256	CB	SER A	93	3.171	35.909	5.763	1.00	74.91
	2257	OG	SER A	93	2.111	36.461	6.531	1.00	74.91
	2258	С	SER A	93	1.912	33.019	4.956	1.00	55.78
25	2259	0	SER A	93	2.205	32.828	4.501 5.796	1.00 1.00	55.78 63.55
	2260	N CA	ALA A ALA A	94 94	0.904 0.070	34.112 33.021	6.287	1.00	63.55
	2261 2262	CB	ALA A	94	0.410	32,712	7.734	1.00	137.30
	2263	C	ALA A	94	-1.392	33.445	6.162	1.00	63.55
30	2264	ŏ	ALA A	94	-1.713	34.616	6.341	1.00	63.55
	2265	N	GLU A	95	-2.283	32.501	5.856	1.00	58.25
	2266	CA	GLU A	95	-3.702	32.826	5.684	1.00	58.25 138.90
	2267	CB	GLU A	95 05	-4.344 -3.695	31.866 31.890	4.701 3.337	1.00 1.00	138.90
35	2268 2269	CG CD	GLU A	95 9 5	-3.693 -4.541	31.214	2.269	1.00	138.90
))	2270	OE1	GLU A	95 .	-4.085	31.137	1.108	1.00	138.90
	2271	OE2	GLU A	95	-5.664	30.763	2.584	1.00	138.90
	2272	С	GLU A	95	-4.494	32.844	6.979	1.00	58.25
40	2273	0	GLU A	95	-5.600	33.361	7.016	1.00	58.25
40	2274	N	VAL A	96	-3.934 -4.584	32.267 32.253	8.040 9.353	1.00 1.00	62.67 62.67
	2275 2276	CA CB	VAL A VAL A	96 96	- 	30.912	9.637	1.00	62.13
	2277	CG1	VAL A	96	-6.169	31.021	10.762	1.00	62.13
	2278	CG2	VAL A	96	-5.835	30.401	8.402	1.00	62.13
45	2279	С	VAL A	96	-3.512	32.568	10.386	1.00	62.67
	2280	0	VAL A	96	-2.422	31.999	10.335	1.00	62.67
	2281	N	VAL A	97	-3.829 -2.833	33.449 33.902	11.333 12.289	1.00 1.00	50.85 50.55
	2282 2283	CA CB	VAL A VAL A	97 97	-2.307	35.276	11.860	1.00	70.57
50	2284	CG1	VAL A	97	-1.069	35.609	12.633	1.00	70.57
50	2285	CG2	VAL A	97	-2.063	35.319	10.372	1.00	70.57
	2286	C	VAL A	97	-3.285	34.077	13.723	1.00	50.85
	2287	0	VAL A	97	-4.373	34.653	13.953	1.00	50.85
	2288	N	MET A	98	-2.449	33.629	14.673	1.00 1.00	73.49 73.49
55	2289	CA CB	MET A	98 98	-2.749 -1.766	33.780 32.956	16.096 16.916	1.00	73.43 225.40
	2290 2291	CB CB	MET A MET A	98	-1.855	31.478	16.645	1.00	228.45
	2292	SD	MET A	98	-3.227	30.766	17.530	1.00	228.45
	2293	CE	MET A	98	-2.529	30.766	19.195	1.00	228.45
60	2294	С	MET A	98	-2.617	35.276	16.477	1.00	73.49
	2295	o	MET A	98	-1.636	35.921	16.109	1.00	73.49
	2296	N	GLU A	89	-3.595	35.826 37.228	17.202 17.603	1.00 1.00	97.63 97.63
	2297 2298	CA CB	GLU A GLU A	99 99	-3.546 -4.562	37.499	18.710	1.00	188.19
65	2298	ČĠ	GLU A	99	-4.954	38.958	18.826	1.00	188.19
0.5	2300	CD	GLU A	99	-5.707	39.259	20.106	1.00	188.19
	2301	OE1	GLU A	99	-6.524	38.412	20.529	1.00	188.19
	2302	OE2	GLU A	99	-5.492	40.347	20.682	1.00	188.19
70	2303	C	GLU A	99	-2.146	37.510 36.793	18.128	1.00 1.00	97.63 97.63
70	2304	0	GLU A	99	-1.651	36.783	18.987	1.00	ar.03

	2305 2306	N CA	GLY A	100 100	-1.492 -0.159	38.538 38.881	17.594 18.066	1.00 1.00	88.99 88.99
	2307	င်	GLY A	100	0.992	38.577	17.130	1.00	88.99
	2308	ŏ.	GLY A	100	2.071	39.135	17.293	1.00	88.99
5	2309	N	GLN A	101	0.777	37.699	16.154	1.00	57.71
	2310	CA	GLN A	101	1.820	37.329	15.192	1.00	57.71
	2311	CB	GLN A	101	1.568	35.933	14.652	1.00	91.13
	2312	CG CD	GLN A GLN A	101	1.663 2.932	34.861 34.976	15.708 16.532	1.00 1.00	91.13
10	2313 2314	OE1	GLN A	101 101	3.038	35.828	17.420	1.00	91.13 91.13
10	2315	NE2	GLN A	101	3.912	34.131	16.230	1.00	91.13
	2316	C	GLN A	101	1.973	38.281	14.017	1.00	57.71
	2317	0	GLN A	101	1.117	39.124	13.763	1.00	57.71
1.5	2318	N	PRO A	102	3.070	38.153	13.266	1.00	73.79
15	2319	CD	PRO A	102	4.201	37.220	13.403	1.00	74.96
	2320 2321	CA CB	PRO A PRO A	102 102	3.264 4.760	39.049 38.932	12.130 11.873	1.00 1.00	73.79 74.96
	2322	CG	PRO A	102	5.018	37.499	12.139	1.00	74.96
	2323	Č	PRO A	102	2.425	38.610	10.940	1.00	73.79
20	2324	O	PRO A	102	2.053	37.446	10.831	1.00	73.79
	2325	N .	LEU A	103	2.125	39.551	10.054	1.00	77.13
	2326	CA	LEU A	103	1.345	39.258	8.862	1.00	77.13
	2327 2328	CB CG	LEU A LEU A	103 103	-0.101 -0.892	39.627 39.326	9.094 7.8 3 1	1.00 1.00	77.95 77.95
25	2329	CD1	LEU A	103	-0.843	37.836	7.584	1.00	77.95
20	2330	CD2	LEU A	103	-2.324	39.799	7.975	1.00	77.95
	2331	C	LEU A	103	1.850	40.060	7.680	1.00	77.13
	2332	0	LEU A	103	1.892	41.280	7.769	1.00	77.13
30	2333	N	PHE A	104	2.226	39.404	6.580	1.00	65.06
30	2334 2335	CA CB	PHE A PHE A	104 104	2.708 4.175	40.147 39.821	5.410 5.102	1.00 1.00	65.06
	2336	CG	PHE A	104	5.118	40.096	6.246	1.00	119.06 119.06
	2337	CD1	PHE A	104	5.209	39.208	7.312	1.00	119.06
	2338	CD2	PHE A	104	5.926	41.237	6.255	1.00	119.06
35	2339	CE1	PHE A	104	6.086	39.443	8.379	1.00	119.06
	2340	CE2	PHE A	104	6.811	41.486	7.321	1.00	119.06
	2341 2342	CZ C	PHE A PHE A	104 104	6.891 1.869	40.585 39.886	8.382 4.164	1.00 1.00	119.06 65.06
	2343	ŏ	PHE A	104	1.640	38.741	3.816	1.00	65.06
40	2344	Ň	LEU A	105	1.373	40.944	3.519	1.00	48.39
	2345	CA	LEU A	105	0.597	40.795	2.282	1.00	48.39
	2346	CB	LEU A	105	-0.708	41.544	2.354	1.00	38.52
	2347	CG	LEU A LEU A	105	-1.516	41.145	3.570	1.00	38.52
45	2348 2349	CD1 CD2	LEU A LEU A	105 105	-2.952 -1.587	41.785 39.647	3.515 3.571	1.00 1.00	38.52 38.52
13	2350	C	LEU A	105	1.445	41.417	1.205	1.00	48.39
	2351	ō	LEU A	105	2.137	42.397	1.461	1.00	48.39
	2352	N	ARG A	106	1.385	40.872	0.001	1.00	64.12
50	2353	CA	ARG A	106	2.198	41.394	-1.074	1.00	64.12
50	2354 2355	CB CG	ARG A	106 106	3.424	40.501	-1.232 -2.370	1.00	100.28
	2356	CD	ARG A ARG A	106	4.313 5.351	40.873 39.801	-2.607	1.00 1.00	100.28 100.28
	2357	NE	ARG A	106	6.190	40.124	-3.755	1.00	100.28
	2358	CZ	ARG A	106	6.892	39.234	-4.443	1.00	100.28
55	2359	NH1	ARG A	106	6.854	37.957	-∕ ₁ .100	1.00	100.28
	2360	NH2	ARC 4	106	7.619	39.623	-5.484	1.00	100.28
	2361	C	ARG A	106	1.416	41.451	-2.380 2.700	1.00	64.12
	2362 2363	N	ARG A CYS A	106 107	0.842 1.349	40.444 42.619	-2. 799 -3.018	1.00 1.00	64.12 99.13
60	2364	ĞA	CYS A	107	0.651	42.685	-4.301	1.00	99.13
•	2365	C	CYS A	107	1.710	42.307	-5.317	1.00	99.13
	2366	0	CYS A	107	2.639	43.059	-5.575	1.00	99.13
	2367	CB	CYS A	107	0.113	44.075	-4.597	1.00	103.70
65	2368	SG	CYS A	107	-1.146	44.090	-5.916	1.00	103.70
U.S	2369 2370	N CA	HIS A HIS A	108 108	1.573 2.530	41.112 40.575	-5.866 -6.804	1.00 1.00	72.29 72.29
	2371	CB	HIS A	108	2.799	39.131	-6.429	1.00	116.05
	2372	ÇG	HIS A	108	3.921	38.508	-7.191	1.00	116.05
~ ^	2373	CD2	HIS A	108	3.973	37.391	-7.950	1.00	116.05
70	2374	ND1	HIS A	108	5.195	39.028	-7.190	1.00	116.05

	2375	CE1	HIS A	108	5.986	38.256	-7.913	1.00	116.05
	2376	NE2	HIS A	108	5.268	37.255	-8.385	1.00	116.05
	2377	Ç .	HIS A	108	2.119	40.651	-8 <i>.2</i> 71	1.00	72.29
5	2378	0	HIS A	108	1.045	40.176	-8.674	1.00	72.29
3	2379 2380	N CA	GLY A	109	2.999	41.242	-9.070	1.00	118.98
	2381	CA C	GLY A	10 9 109	2.7 3 5 3.202	41.367 40.136	-10.485	1.00	118.98
	2382	ŏ	GLY A	109	4.083	39.410	-11.231 -10.772	1.00	118.98
	2383	Ň	TRP A	110	2.603	39.894	-12.389	1.00 1.00	118.98
10	2384	CA	TRP A	110	2.968	38.751	-13.202	1.00	106.09 106.09
	2385	CB	TRP A	110	2.016	38.629	-14.395	1.00	134.90
	2386	CG	TRP A	110	2.418	37.581	-15.361	1.00	134.90
	2387	CD2	TRP A	110	1.980	36.223	-15.380	1.00	134.90
	2388	CE2	TRP A	110	2.657	35.576	-16.431	1.00	134.90
15	2389	CE3	TRP A	110	1.072	35.481	-14.604	1.00	134.90
	2390	CD1	TRP A	110	3.314	37.707	-16.370	1.00	134.90
	2391	NE1	TRP A	110	3.466	36.509	-17.021	1.00	134.90
	2392 2393	CZ2 CZ3	TRP A	110	2.464	34.224	-16.732	1.00	134.90
20	2394	CH2	TRP A	110 110	0.879 1.575	34.132 33.521	-14.905	1.00	134.90
20	2395	C	TRP A	110	4.399	38.899	-15.958 -13.683	1.00 1.00	134.90 106.09
	2396	ŏ	TRP A	110	4.916	40.008	-13.825	1.00	106.09
	2397	Ň	ARG A	111	5.043	37.764	-13.918	1.00	87.25
	2398	CA	ARG A	111	6.426	37.750	-14.392	1.00	87.25
25	2399	CB	ARG A	111	6.468	38.086	-15.858	1.00	235.25
	2400	CG	ARG A	111	6.316	36.881	-16.692	1.00	235.25
	2401	CD	ARG A	111	6.642	37.245	-18.072	1.00	235.25
	2402	NE	ARG A	111	7.428	36.197	-18.691	1.00	235.25
30	2403	CZ	ARG A	111	8.674	35.887	-18.358	1.00	235.25
50	2404 2405	NH1 NH2	ARG A	111 111	9.295	36.552	-17. 39 2	1.00	235.25
	2406	C	ARG A	111	9.290 7.358	34.895 38.697	-18.988 -13.665	1.00	235.25
	2407	ŏ	ARG A	111	8.402	39.105	-13.005 -14.191	1.00 1.00	87.25 87.25
	2408	Ň	ASN A	112	6.964	39.048	-12.453	1.00	105.23
35	2409	CA	ASN A	112	7.744	39.942	-11.633	1.00	105.23
	2410	СВ	ASN A	112	9.121	39.353	-11.375	1.00	116.08
	2411	CG	ASN A	112	9.735	39.907	-10.118	1.00	116.08
	2412	OD1	ASN A	112	9.369	41.000	-9.660	1.00	116.08
40	2413	ND2	ASN A	112	10.668	39.166	-9.544	1.00	116.08
40	2414 2415	C O	ASN A	112	7.905	41.345	-12.218	1.00	105.23
	2416	N	ASN A TRP A	112 113	8.852 6.992	42.055 41.753	-11.885	1.00	105.23
	2417	ĞA	TRP A	113	7.095	43.088	-13.089 -13.645	1.00 1.00	124.66 124.66
	2418	CB	TRP A	113	6.019	43.344	-14.688	1.00	167.38
45	2419	CG	TRP A	113	6.315	42.730	-15.979	1.00	167.38
	2420	CD2	TRP A	113	5.379	42.134	-16.868	1.00	167.36
	2421	CE2	TRP A	113	6.091	41.718	-18.006	1.00	167.38
	2422	CE3	TRP A	113	3.997	41.914	-16.816	1.00	167.38
50	2423	CD1	TRP A	113	7.533	42.658	-16.592	1.00	167.38
20	2424	NE1	TRP A	113	7.406	42.049	-17.813	1.00	167.38
	2425 2426	CZ2 CZ3	TRP A	113	5.475	41.093	-19.080	1.00	167.38
	2427	CH2	TRP A	113 113	3,383	41.293	-17.886	1.00	167.38
	2428	C	TRP A	113	4.126 6.939	40.886 44.106	-19.004 -12.540	1.00 1.00	167.38
55	2429	ŏ	TRP A	113	6.964	43.768	-11.357	1.00	124.66 124.66
	2430	Ň	ASP A	114	6.773	45.359	-12.937	1.00	183.63
	2431	CA	ASP A	114	6.603	46.430	-11.981	1.00	183.83
	2432	CB	ASP A	114	7.598	47.558	-12.258	1.00	145.30
60	2433	CG	ASP A	114	8.978	47.26 9	-11.692	1.00	145.30
60	2434	OD1	ASP A	114	9.077	47.087	-10.459	1.00	145.30
	2435	OD2	ASP A	114	9.957	47.225	-12.473	1.00	145.30
	2436 2437	C	ASP A ASP A	114	5.188	46.956 47.108	-12.034	1.00	183.83
	2437 2438	Ň	VAL A	114 115	4.598 4.645	47.106 47.218	-13.108 -10.853	1.00	183.83
65	2439	CA CA	VAL A	115	3.294	47.216 47.740	-10.853 -10.735	1.00 1.00	117.62 117.82
	2440	CB	VAL A	115	2.421	46.835	-10.735 -9.879	1.00	77.28
	2441	CG1	VAL A	115	0.971	47.248	-10.008	1.00	77.28
	2442	CG2	VAL A	115	2.616	45.409	-10.302	1.00	77.28
70	2443	C	VAL A	115	3.329	49.116	-10.089	1.00	117.62
70	2444	0	VAL A	115	4.142	49.377	-9.191	1.00	117.62

	2445	N	TYR /		2.444	49.995	-10.553	1.00	77.55
	2446	CA	TYR /		2.380	51.344	-10.021	1.00	77.55
	2447 2448	CB CG	TYR A		2.831 4.271	52.352 52.172	-11.086	1.00	167.00
5	2449	CD1	TYR A		4.581	52.172 51.453	-11.532 -12.676	1.00	167.00
_	2450	CE1	TYR A		5.909	51.265	-13.071	1.00 1.00	167.00
	2451	CD2	TYR A		5.325	52.793	-10.789	1.00	167.00 167.00
	2452	CE2	TYR A		6.653	52.519	-11.173	1.00	167.00
10	2453	CZ	TYR A		6.937	51.800	-12.312	1.00	167.00
10	2454	ОН	TYR A		8.246	51.606	-12.687	1.00	167.00
	2455 2456	C	TYR A		0.984	51.699	·9.519	1.00	77.55
	2457	N	LYS		0. 023 0. 879	50.951 52.842	-9.742 -8.840	1.00	77.55
	2458	ČA	LYS A		-0.399	53.292	-8.310	1.00 1.00	94.85
15	2459	CB	LYS A		-1.300	53.834	-9.423	1.00	94.85 193.46
	2460	CG	LYS A	A 117	-1.084	55.291	-9.786	1.00	193.46
	2461	CD	LYS A		-2.284	55.824	-10.563	1.00	193.46
	2462	CE	LYS A		-3.569	55.726	-9.735	1.00	193.46
20	2463 2464	NZ C	LYS A		-4.780	56.210	-10.464	1.00	193.46
20	2465	ŏ	LYS A		-1.099 -2.226	52.125 51.770	-7.629 -7.977	1.00	94.85
	2466	Ň	VAL A		-0.422	51.530	-6. 65 5	1.00 1.00	94.85 105.41
	2467	CA	VAL A	118	-0.979	50.402	-5.927	1.00	105.41
05	2468	CB	VAL A		0.122	49.503	-5.445	1.00	73.04
25	2469	CG1	VAL A		-0.314	48.777	-4.205	1.00	73.04
	2470 2471	CG2 C	VAL A		^ 455	48.521	-6.514	1.00	73.04
	2472	ŏ	VAL A		-1.862 -1.527	50.736	-4.723 2.004	1.00	105.41
	2473	Ň	ILE A		-1.527 -2.971	51.582 50.020	-3.894 -4.607	1.00	105.41
30	2474	CA	ILE A		-3.902	50.248	-3.518	1.00 1.00	71.97 71.97
	2475	СВ	ILE A		-5.125	51.002	-4.016	1.00	77.41
	2476	CG2	ILE A		-6.037	51.319	-2.866	1.00	77.41
	2477	CG1	ILE A		-4.687	52.285	-4.705	1.00	77.41
35	2478 2479	CD1 C	ILE A		-5.804	52.949	-5.467	1.00	77.41
33	2480	ŏ	ILE A		-4.395 -4.954	48.928 48.146	-2.961 -3.701	1.00	71.97
	2481	Ň	TYR A		-4.193	48.654	-1. 679	1.00 1.00	71.97 64.29
	2482	CA	TYR A		-4.698	47.403	-1.117	1.00	64.29
40	2483	СВ	TYR A		-3.867	46.908	0.059	1.00	49.60
40	2484	CG	TYR A		-2.521	46.438	-0.297	1.00	49.60
	2485 2486	CD1 CE1	TYR A		-1.472	47.324	-0.395	1.00	49.60
	2487	CD2	TYR A		-0.195 -2.292	46.897 45.109	-0. 73 6 -0. 54 6	1.00	49.60
	2488	CE2	TYR A		-1.026	44.650	-0.901	1.00 1.00	49.60 49.60
45	2489	CZ	TYR A		0.020	45.548	-0.992	1.00	49.60 49.60
	2490	OH	TYR A		1.268	45.095	-1.339	1.00	49.60
	2491	C	TYR A		-6.069	47.879	-0.580	1.00	64.29
	2492 2493	0	TYR A		-6.313	48.764	-0.069	1.00	64.29
50	2483 2484	N CA	TYR A		-6.945 -8.299	46.686	-0.658	1.00	62.29
•	2495	CB	TYR A		-9.315	46. 83 8 46.752	-0.154 -1.302	1.00 1.00	62.29
	2496	ČĠ	TYR A		-9.308	47,900	-2.293	1.00	87.89 87.89
	2497	CD1	TYR A	121	-8.219	48.119	-3.126	1.00	87.89
55	2498	CE1	TYR A		-8.232	49.147	-4.073	1.00	87.89
55	2499	CD2	TYR A		-10.422	48.745	-2.424	1.00	87.89
	2500 2501	CE2 CZ	TYR A		-10.450	49.776	-3.368	1.00	87.89
	2502	OH OH	TYR A		-9.351 -9.383	49.970 50.966	-4.193 -5.150	1.00	37.89
	2503	Č	TYR A		-8.647	45.772	-5.156 0.883	1.00 1.00	87.89 62.29
60	2504	0	TYR A		-8.275	44.598	0.723	1.00	62.29
	2505	N	LYS A		-9.349	46.180	1.943	1.00	53.98
	2506	CA	LYS A		-9.794	45.238	2.957	1.00	53.98
	2507 2508	CB	LYS A		-9.069	45.436	4.278	1.00	98.53
65	2508 2509	CG CD	LYS A		-9.499 -9.038	44.427	5.329	1.00	98.53
	2510	CE	LYS A		-9.644	44.809 43.912	6.719 7.774	1.00	98.53
	2511	NZ	LYS A		-9.317	44.426	9.120	1.00 1.00	98.53 98.53
	2512	Ç	LYS A	122	-11.291	45.452	3.158	1.00	53.98
70	2513	0	LYS A		-11.720	46.526	3.569	1.00	53.98
70	2514	N	ASP A	123	-12.081	44.429	2.841	1.00	82.84

	2515	CA	ASP A	123	-13.530	44,491	2.976	1 00	00.04
	2516	CB	ASP A	123	-13.926	44,624	4.449	1.00 1.00	82.84
	2517	ČĠ	ASP A	123	-13.786	43.313	5.204	1.00	104.85
	2518	OD1	ASP A	123	-14.244	42.269	4.680	1.00	104.85
5	2519	OD2	ASP A	123	-13.228	43.321	6.324	1.00	104.85 104.85
-	2520	C	ASP A	123	-14.140	45.620	2.158	1.00	82.84
	2521	ŏ	ASP A	123	-15.013	46.350	2.638	1.00	82.84
	2522	N	GLY A	124	-13.677	45.743	0.915	1.00	89.57
	2523	CA	GLY A	124	-14.179	46.772	0.018	1.00	89.57
10	2524	С	GLY A	124	-13.699	48.197	0.279	1.00	89.57
	2525	0	GLY A	124	-13.981	49.093	-0.528	1.00	89.57
	2526	N	GLU A	125	-12.978	48.412	1.382	1.00	81.16
	2527	CA	GLU A	125	-12.476	49.746	1.745	1.00	81.16
	2528	СВ	GLU A	125	-12.470	49.925	3.274	1.00	176.94
15	2529	CG	GLU A	125	-13.834	49.988	3.958	1.00	176.94
	2530	CD	GLU A	125	-14.499	51.350	3.844	1.00	176.94
	2531	OE1	GLU A	125	-13.931	52.343	4.352	1.00	176.94
	2532	OE2	GLU A	125	-15.595	51.428	3.251	1.00	176.94
20	2533	C	GLU A	125	-11.055	50.008	1.238	1.00	81.16
20	2534	0	GLU A	125	-10.223	49.116	1.229	1.00	81.16
	2535	N	ALA A	126	-10.772	51.228	0.815	1.00	92.74
	2536	CA	ALA A	126	-9.424	51.546	0.375	1.00	92.74
	2537	СВ	ALA A	126	-9.379	52.967	-0.145	1.00	165.28
25	2538 2539	C O	ALA A	126	-8.592	51.410	1.650	1.00	92.74
23	2540	N	ALA A LEU A	126	-9.083	51.719	2.731	1.00	92.74
	2540 2541	ČA	LEU A	127 127	-7.347	50.957	1.550	1.00	58.95
	2542	CB	LEU A	127	-6.544 -6.333	50.778	2.749	1.00	58.95
	2543	CG	LEU A	127	-6.046	49.305	3.037	1.00	73.14
30	2544	CD1	LEU A	127	-7.224	49.150 49.745	4.528 5.285	1.00 1.00	73.14
50	2545	CD2	LEU A	127	-5.840	47.693	4.917	1.00	73.14
	2546	C	LEU A	127	-5.195	51.457	2.764	1.00	73.14
	2547	ŏ	LEU A	127	-4.910	52.212	3.691	1.00	58.95 58.95
	2548	Ň	LYS A	128	-4.344	51.153	1.788	1.00	77.17
35	2549	CA	LYS A	128	-3.028	51.788	1.690	1.00	77.17
	2550	CB	LYS A	128	-1.920	50.862	2.197	1.00	133.78
	2551	CG	LYS A	128	-2.041	50.465	3.656	1.00	133.78
	2552	CD	LYS A	128	-1.716	51.601	4.605	1.00	133.78
40	2553	CE	LYS A	128	-1.741	51.120	6.052	1.00	133,78
40	2554	NZ	LYS A	128	-1.293	52.157	7.033	1.00	133.78
	2555	C	LYS A	128	-2.788	52.130	0.212	1.00	77.17
	2556	0	LYS A	128	-3.348	51.493	-0.675	1.00	77.17
	2557 2558	N	TYR A	129	-1.973	53.142	-0.063	1.00	64.91
45	2559	CA CB	TYR A	129 129	-1.693	53.519	-1,444	1.00	64.91
73	2560	ca	TYR A	129	-2.633 -2.100	54.637	-1.882	1.00	122.39
	2561	CD1	TYR A	129	-2.100	55.390 54.874	-3. 0 80 -4.366	1.00	122.39
	2562	CE1	TYR A	129	-1.702	54.874 55.539	-5.465	1.00 1.00	122.39
	2563	CD2	TYR A	129	-1.416	56.599	-2.919	1.00	122.39 122.39
50	2584	CE2	TYR A	129	-0.875	57.273	-4.012	1.00	122.39
	2565	CZ	TYR A	129	-1.024	56.738	-5.282	1.00	122.39
	2566	OH	TYR A	129	-0.508	57.402	-6.370	1.00	122,39
	2567	Ċ	TYR A	129	-0.244	53.978	-1.679	1.00	64.91
	2568	0	TYR A	129	0.320	54.739	-0.885	1.00	64.91
55	2569	N	TRP A	130	0.348	53.530	-2.787	1.00	121.28
	2570	CA	TRP A	130	1.713	53.914	-3.125	1.00	121.28
	2571	CB	TRP A	130	2.715	52.874	-2.627	1.00	194.88
	2572	CG	TRP A	130	2.557	52.464	-1.196	1.00	194.88
60	2573	CD2	TRP A	130	3.398	52.848	-0.100	1.00	194.88
60	2574	CE2	TRP A	130	2.909	52.182	1.049	1.00	194.88
	2575	CE3	TRP A	130	4.508	53.694	0.023	1.00	194.88
	2576	CD1	TRP A	130	1.629	51.608	-0.683	1.00	194.88
	2577	NE1	TRP A	130	1.833	51.431	0.666	1.00	194.88
65	2578	CZ2	TRP A	130	3.500	52.334	2.309	1.00	194.88
UJ	2579	CZ3	TRP A	130	5.096	53.847	1.280	1.00	194.88
	2580	CH2	TRP A	130	4.592	53.163	2.403	1.00	194.88
	2581 2582	C	TRP A	130	1.907	54.064 F2 607	-4.627 5.400	1.00	121.28
	2583	Ň	TRP A	130	1.075	53.627	-5.422 -5.015	1.00	121.28
70	2584	CA	TYR A	131 131	3.015 3.304	54.685 54.849	-5.015 -6.426	1.00	100.84
		-	TIO A	101	3.304	34.048	-6.426	1.00	100.84

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	2585 2586	CB CG	TYR A TYR A	131	4.202	56.059	-6.683	1.00	199.69
	2587	CD1	TYR A	131 131	4.299 3.223	56.369 56.944	-8.155	1.00	199.69
	2588	CE1	TYR A	131	3.246	57.115	-8.830 -10.206	1.00	199.69
5	2589	CD2	TYR A	131	5.414	55.982	-8.899	1.00 1.00	199.69
	2590	CE2	TYR A	131	5.448	56.148	-10.281	1.00	199.69 199.69
	2591	CZ	TYR A	131	4.357	56.712	-10.926	1.00	199.69
	2502	OH	TYR A	131	4.364	56.843	-12.295	1.00	199.69
10	2593	Ç	TYR A	131	4.029	53.572	-6 .818	1.00	100.84
10	2594	0	TYR A	131	3.397	52.644	-7.326	1.00	100.84
	2595	N CA	GLU A	132	5.351	53.543	-6.624	1.00	218.16
	2596 2597	CA CB	GLU A GLU A	132	6.122	52. 331	-6.894	1.00	218.16
	2598	CG	GLU A	132 132	7.629 8.382	52.547 53.317	-6.666 7.760	1.00	249.55
15	2599	CD	GLU A	132	9.480	52.4 82	-7.762 -8.422	1.00 1.00	249.55
	2600	OE1	GLU A	132	9.903	51.469	-7.822	1.00	249.55 249.55
	2601	OE2	GLU A	132	9.922	52.848	-9.533	1.00	249.55
	2602	С	GLU A	132	5.531	51. 536	-5.747	1.00	218.16
20	2603	0	GLU A	132	5.514	52.022	-4.616	1.00	218.16
20	2604	N	ASN A	133	5.032	50.334	-6.012	1.00	155.99
	2605 2606	CA CB	ASN A ASN A	133	4.388	49.588	-4.939	1.00	155.99
	2607	CG	ASN A	133 133	3.656 4.538	48.353 47.157	-5.472	1.00	108.04
	2608	OD1	ASN A	133	5.620	47.137 47.230	-5.575 -6.143	1.00 1.00	108.04
25	2609	ND2	ASN A	133	4.085	46.035	-5.035	1.00	108.04 108.04
	2610	С	ASN A	133	5.244	49.194	-3.759	1.00	155.99
	2611	0	ASN A	133	6.458	49.376	-3.734	1.00	155.99
	2612	N	HIS A	134	4.560	48.629	-2.779	1.00	115.35
30	2613	CA	HIS A	134	5.153	48.235	-1.520	1.00	115.35
30	2614 2615	CB	HIS A	134	4.782	49.305	-0.489	1.00	200.02
	2616	CD2	HIS A HIS A	134 134	5.436	49.129	0.842	1.00	200.02
	2617	ND1	HIS A	134	4.912 6.799	48.8 9 3 49.213	2.067 1.016	1.00 1.00	200.02
	2618	CE1	HIS A	134	7.088	49.035	2.293	1.00	200.02 200.02
35	2619	NE2	HIS A	134	5.961	48.840	2.951	1.00	200.02
	2620	C	HIS A	134	4.596	46.874	-1.114	1.00	115.35
	2621	O.	HIS A	134	4.008	46.161	-1.934	1.00	115.35
	2622 2623	N CA	ASN A ASN A	135	4.781	46.524	0.153	1.00	81.38
40	2624	CB	ASN A	135 135	4.298 5.426	45. 263 . 44. 243	0.675	1.00	81.38
	2625	ČĠ	ASN A	135	5.832	43.891	0.654 -0.754	1.00 1.00	168.37
	2626	OD1	ASN A	135	4.964	43.656	-1.596	1.00	168.37 168.37
	2627	ND2	ASN A	135	7.134	43.839	-1.029	1.00	168.37
AE	2628	C	ASN A	135	3.748	45.431	2.073	1.00	81.38
45	2629	0	ASN A	135	4.455	45.219	3.042	1.00	81.38
	2630 2631	N CA	ILE A ILE A	136	2.481	45.817	2.168	1.00	68.07
	2632	CB	ILE A	136 136	1.826 0.288	46.032 46.019	3.456	1.00	68.07
	2633	CG2	ILE A	136	-0.135	44.814	3.287 2.531	1.00 1.00	88.63
50	2834	CG1	ILE A	136	-0.397	46.040	4.638	1.00	86.88 86.88
	2635	CD1	ILE A	136	-1.885	46.136	4.514	1.00	36.88
	2636	C	ILE A	136	2.277	44.997	4.482	1.00	68.07
	2637	O.	ILE A	136	2.085	43.801	4.301	1.00	68.07
55	2638 2639	N CA	SER A	137	2.904	45.484	5.550	1.00	113.35
55	2640	CA CB	SER A SER A	137 137	3.422	44.631	6.606	1.00	113.35
	2641	og	SER A	137	4.932 5.433	44.798 44.258	6.686	1.00	. 0.04
	2642	C	SER A	137	2.808	44.903	7.891 7.974	1.00 1.00	73.04 113.35
	2643	0	SER A	137	2.469	46.029	8.304	1.00	113.35
60	2644	N	ILE A	138	2.688	43.856	8.777	1.00	71.19
	2645	CA	ILE A	138	2.116	43.961	10.117	1.00	71.19
	2646	CB	ILE A	138	0.715	43.413	10.147	1.00	41.44
	2647 2648	CG2 CG1	ILE A	138	0.257	43.304	11.582	1.00	41.44
65	2649	CD1	ILE A ILE A	138 138	-0.212 -1.531	44.297 43.837	9.318	1.00	41.44
	2650	Č.	ILE A	138	2.922	43.627 43.170	9.019 11.146	1.00 1.00	41.44
	2651	Ŏ	ILE A	138	3.093	41.954	11.012	1.00	71.19 71.19
	2652	N	THR A	139	3.397	43.856	12.185	1.00	108.53
70	2653	CA	THR A	139	4.195	43.216	13.234	1.00	108.53
70	2654	СВ	THR A	139	5.001	44.260	14.012	1.00	232.49

	2655	OG1	THR A	120	. 4 107	45.004	44.400		
	2656	CG2	THR A	139 139	4.127 6.080	45.304 44.854	14.460	1.00	232.49
	2657	C	THR A	139	3.291	44.854 42.458	13.121	1.00	232.49
	2658	ŏ	THR A	139	3.199	41.235	14.192 14.125	1.00	108.53
5	2659	Ň	ASN A	140	2.632	43.192	15.083	1.00 1.00	108.53
	2660	CA	ASN A	140	1.699	42.621	16.050	1.00	125.42
	2661	CB	ASN A	140	1.662	43.455	17.328	1.00	125.42 148.98
	2662	CG	ASN A	140	0.619	42.967	18.305	1.00	148.98
10	2663	OD1	ASN A	140	-0.533	42.738	17.950	1.00	148.98
10	2664	ND2	ASN A	140	1.024	42.828	19.558	1.00	148.98
	2665	C	ASN A	140	0.335	42.677	15.375	1.00	125.42
	2666	0	ASN A	140	-0.149	43.763	15.030	1.00	125.42
	2667 2668	N	ALA A	141	-0.291	41.518	15.203	1.00	57.61
15	2669	CA CB	ALA A ALA A	141	-1.569	41.462	14.527	1.00	57.61
13	2670	C	ALA A ALA A	141 141	-1.605	40.246	13.644	1.00	27.12
	2671	ŏ	ALA A	141	-2.785 -2.895	41.468 40.661	15.439	1.00	57.61
	2672	Ň	THR A	142	-3.713	42.373	16.364	1.00	57.61
	2673	CA	THR A	142	-4.939	42.481	15.149 15.912	1.00	70.60
20	2674	СВ	THR A	142	-5.488	43.5 J	15.811	1.00 1.00	70.60
	2675	OG1	THR A	142	-4.440	44.833	16.136	1.00	136.27
	2676	CG2	THR A	142	-6.643	44.104	16.773	1.00	136.27 136.27
	2677	С	THR A	142	-5.937	41.478	15.334	1.00	70.60
25	2678	0	THR A	142	-5.666	40.852	14.311	1.00	70.60
25	2679	N	VAL A	143	-7.066	41.285	16.001	1.00	71.67
	2680	CA	VAL A	143	-8.057	40.355	15.489	1.00	71.67
	2681	CB	VAL. A	143	-8.949	39.782	16.610	1.00	65.94
	2682 2683	CG1	VAL A	143	-9.785	40.880	17.217	1.00	65.94
30	2684	CG2 C	VAL A	143	-9.848	38.672	16.047	1.00	65.94
50	2685	ŏ	VAL A	143	-8.934	41.126	14.518	1.00	71.67
	2686	Ň	GLU A	143 144	-9.679 -8.842	40.552 42.442	13.726	1.00	71.67
	2687	ČA	GLU A	144	-9.650	42. 44 2 43.260	14.579 13.699	1.00	71.12
	2688	CB	GLU A	144	-9.747	44.691	14.235	1.00 1.00	71.12
35	2689	CG	GLU A	144	-10.475	44.796	15.566	1.00	228.43 228.43
	2690	CD	GLU A	144	-9.558	45.204	16.699	1.00	228.43
	2691	OE1	GLU A	144	-8.966	46.296	16.611	1.00	228.43
	2692	QE2	GLU A	144	-9.428	44.440	17.676	1.00	228.43
40	2693	C	GLU A	144	-9.068	43.250	12.301	1.00	71.12
40	2694	0	GLU A	144	-9.732	43.609	11.338	1.00	71.12
	2695 2696	N CA	ASP A	145	-7.821	42.820	12.194	1.00	58.24
	2697	CB	ASP A	145 145 -	-7.146	42.754	10.900	1.00	58.24
	2698	CG	ASP A	145	-5.645 -4.945	42.541 42.704	11.091	1.00	106.20
45	2699	OD1	ASP A	145	-5.013	43.784 44.817	11.606	1.00	106.20
	2700	OD2	ASP A	145	-4.329	43.733	10.911 12.696	1.00 1.00	106.20
	2701	C	ASP A	145	-7.705	41.643	10.018	1.00	106.20 58.24
	2702	0	ASP A	145	-7.434	41.608	8.819	1.00	58.24 58.24
	2703	N	SER A	146	-8.490	40.744	10.607	1.00	85.01
50	2704	CA	SER A	146	-9.077	39.652	9.848	1.00	85.01
	2705	CB	SER A	146	-9.781	38.669	10.789	1.00	118.46
	2706	og.	SER A	146	-8.854	38.089	11.691	1.00	118.46
	2707 2709	C	SER A	146	-10.052	40.266	8.855	1.00	85.01
55	2708 2709	0	SER A	146	-10.741	41.227	9.168	1.00	85.01
55	2710	N CA	GLY A	147	-10.081	39.735	7.644	1.00	64.55
	2711	č	GLY A	147 147	-10.972	40.264	6.632	1.00	64.55
	2712	ŏ	GLY A	147	-10.649 -9.963	39.664 38.628	5.277	1.00	64.55
	2713	Ň	THR A	148	-11.147	40.285	5.214 4.201	1.00	64.55
60	2714	CA	THR A	148	-10.881	39.795	2.841	1.00 1.00	54.60
	2715	CB	THR A	148	-12.159	39.339	2.143	1.00	54.60 77.82
	2716	OG1	THR A	148	-12,541	40.316	1.193	1.00	77.82
	2717	CG2	THR A	148	-13.272	39.179	3.148	1.00	77.82
65	2718	Ç	THR A	148	-10.204	40.891	2.029	1.00	54.60
65	2719	0	THR A	148	-10.789	41.941	1.746	1.00	54.60
	2720	N OA	TYR A	149	-8.958	40.639	1.661	1.00	38.49
	2721	CA CB	TYR A	149	-8.181	41.622	0.950	1.00	38.49
	2722 2723	CB CB	TYR A	149	-6.775	41.604	1.518	1.00	47.71
70	2724	CD1	TYR A TYR A	149 149	-6.654 -7.129	41.954	2.987	1.00	47.71
. •			1111 M	148	-7.128	41.123	3.982	1.00	47.71

	2725 2726 2727	CE1 CD2 CE2	TYR A TYR A TYR A	149 149 149	-6.952 -6.010 -5.832	41.468 43.124 43.470	5.327 3.370 4.691	1.00 1.00 1.00	47.71 47.71
5	2728 2729 2730 2731	CZ OH	TYR A TYR A TYR A TYR A	149 149 149	-6.297 -6.098 -8.098	42.656 43.066 41.368	5.669 6.973 -0.543	1.00 1.00 1.00	47.71 47.71 47.71 38.49
10	2732 2733 2734	N CA CB	TYR A TYR A TYR A	149 150 150 150	-8.451 -7.639 -7.385 -8.681	40.272 42.382 42.305 42.142	-1.006 -1.279 -2.716 -3.520	1.00 1.00 1.00 1.00	38.49 53.38 53.38
	2735 2736 2737 2738	CG CD1 CE1	TYR A TYR A TYR A	150 150 150	-9.564 -9.167 -9.992	43.353 44.393 45.488	-3.735 -4.563 -4.795	1.00 1.00 1.00	86.43 86.43 86.43 86.43
15	2739 2740 2741	CD2 CE2 CZ OH	TYR A TYR A TYR A TYR A	150 150 150 150	-10.816 -11.652 -11.234 -12.049	43.436 44.522 45.547 46.642	-3.142 -3.365 -4.190 -4.381	1.00 1.00 1.00 1.00	86.43 86.43 86.43 86.43
20	2742 2743 2744 2745	C O N CA	TYR A TYR A CYS A CYS A	150 150 151 151	-6.653 -6.726 -5.900 -5.179	43.598 44.536 43.660 44.894	-3.028 -2.225 -4.127	1.00 1.00 1.00	53.38 53.38 73.39
25	2746 2747 2748	C O CB	CYS A CYS A CYS A	151 151 151	-5.388 -5.741 -3.680	45.311 44.487 44.745	-4.462 -5.900 -6.721 -4.197	1.00 1.00 1.00 1.00	73.39 73.39 73.39 73.27
23	2749 2750 2751 2752	SG N CA CB	CYS A THR A THR A THR A	151 152 152 152	-2.861 -5.177 -5.335 -6.478	43.358 46.593 47.121 48.154	-5.059 -6.192 -7.537 -7.602	1.00 1.00 1.00	73.27 98.75 98.75
30	2753 2754 2755 2756	OG1 CG2 C O	THR A THR A THR A	152 152 152	-6.138 -7.746 -4.025	49.310 47.558 47.793	-6.821 -7.048 -7.905	1.00 1.00 1.00 1.00	109.76 109.76 109.76 98.75
35	2757 2758 2759 2760	N CA C	THR A GLY A GLY A GLY A	152 153 153 153	-3.329 -3.681 -2.444 -2.392	48.322 47.764 48.385 48.562	-7.032 -9.188 -9.622 -11.122	1.00 1.00 1.00 1.00	98.75 91.16 91.16 91.16
40	2761 2762 2763	O N CA CB	GLY A LYS A LYS A LYS A	153 154 154 154	-3.163 -1.488 -1.359 -1.229	47.947 49.409 49.643 51.140	-11.843 -11.597 -13.023 -13.299	1.00 1.00 1.00 1.00	91.16 71.11 71.11 173.07
40	2764 2765 2766 2767	CG CD CE NZ	LYS A LYS A LYS A LYS A	154 154 154 154	-1.235 -1.155 -1.050 -0.857	51.523 53.036 53.490 54.960	-14.769 -14.911 -16.359	1.00 1.00 1.00	173.07 173.07 173.07
45	2768 2769 2770 2771	C O N CA	LYS A LYS A VAL A	154 154 155	-0.120 0.963 -0.289	48.907 49.009 48.128	-16.420 -13.500 -12.900 -14.563	1.00 1.00 1.00 1.00	173.07 71.11 71.11 -35.85
50	2772 2773 2774	CB · CG1 CG2	VAL A VAL A VAL A	155 155 155 155	0.813 0.510 1.673 0.273	47.372 45.884 45.144 45.373	-15.153 -15.201 -15.841 -13.809	1.00 1.00 1.00 1.00	155.85 196.06 196.06 196.06
	2775 2776 2777 2778	C O N CA	VAL A VAL A TRP A TRP A	155 155 156 156	0.960 -0.013 2.187 2.437	47.894 47.951 48.251 48.821	-16.560 -17.309 -16.912	1.00 1.00 1.00	155.85 155.85 136.77
55	2779 2780 2781	CB CG CD2	TRP A TRP A TRP A	156 156 156	1.888 2.584 3.991	47.941 46.701 46.538	-18.215 -19.308 -19.394 -19.596	1.00 1.00 1.00 1.00	136.77 189.17 .59.17 169.17
60	2782 2783 2784 2785 2786	CE2 CE3 CD1 NE1 CZ2	TRP A TRP A TRP A	156 156 156 156	4.260 5.037 2.066 3.053	45.184 47.423 45.478 44.565	-19.532 -19.855 -19.202 -19.283	1.00 1.00 1.00 1.00	169.17 169.17 169.17 169.17
65	2787 2788 2789	CZ3 CH2 C	TRP A TRP A TRP A TRP A	156 156 156 156	5.536 6.293 6.542 1.664	44.634 46.924 45.522 50.102	-19.734 -20.012 -19.971 -18.251	1.00 1.00 1.00 1.00	169.17 169.17 169.17 136.77
<u></u>	2790 2791 2792 2793	O N CA CB	TRP A GLN A GLN A GLN A	156 157 157 157	2.130 0.445 -0.395 -0.133	51.132 50.004 51.166 51.791	-17.775 -18.777 -18.902	1.00 1.00 1.00	136.77 192.06 192.06
70	2794	CG	GLN A	157	1.231	52.449	-20.263 -20.291	1.00 1.00	249.57 249.57

	2795	CD	GLN A	157	1.374	53.420	-19.126	1.00	249.57
	2796	OE1	GLN A	157	0.539	54.293	-18.950	1.00	249.57
	2797	NE2	GLN A	157	2.428	53.271	-18.339	1.00	249.57
5	2798 2799	C	GLN A GLN A	157	-1.873	50.913	-18.673	1.00	192.06
,	2800	Ň	LEU A	157 158	-2.717 -2.181	51.753 49.753	-18.989 -18.108	1.00 1.00	192.06
	2801	ČA	LEU A	158	-3.565	49.394	-17.813	1.00	96.98 96.98
	2802	· CB	LEU A	158	-4.018	48.234	-18.697	1.00	92.50
	2803	CG	LEU A	158	-4.362	48.530	-20.148	1.00	92.50
10	2804	CD1	LEU A	158	-5.577	47.691	-20.496	1.00	92.50
	2805	CD2	LEU A	158	-4.695	50.015	-20.343	1.00	92.50
	2806	C	LEU A	158	-3.758	49.028	-16.345	1.00	96.98
	2807 2808	0 N	LEU A ASP A	158 159	-2.821 -4.983	48.596 49.216	-15.661	1.00	96.98
15	2809	CA	ASP A	159	·5.330	48.925	-15.869 -14.485	1.00 1.00	119.40 119.40
	2810	CB	ASP A	159	-6.442	49.875	-14.018	1.00	201.99
	2811	CG	ASP A	159	-6.096	51.345	-14.236	1.00	201.99
	2812	OD1	ASP A	159	-5.103	51.832	-13.651	1.00	201.99
20	2813	OD2	ASP A	159	-6.823	52.018	-15.000	1.00	201.99
20	2814	C	ASP A	159	-5.793	47.473	-14.334	1.00	119.40
	2815 2816	0 N	ASP A TYR A	159 160	-6.417 5.475	46.919	-15.235	1.00	119.40
	2817	CA	TYR A	160	-5.475 -5.875	46.860 45.481	-13.197 -12.929	1.00 1.00	117.93
	2818	CB	TYR A	160	-4.769	44.503	-13.308	1.00	117.93 127.75
25	2819	CG	TYR A	160	-4.261	44.648	-14.715	1.00	127.75
	2820	CD1	TYR A	160	-3.184	45.483	-14.997	1.00	127.75
	2821	CE1	TYR A	160	-2.707	45.625	-16.277	1.00	127.75
	2822	CD2	TYR A	160	-4.855	43.952	-15.766	1.00	127.75
30	2823 2824	CE2 CZ	TYR A	160	-4.386	44.087	-17.061	1.00	127.75
50	2825	OH	TYR A TYR A	160 160	-3.309 -2.808	44.932 45.145	-17.297 -18.541	1.00 1.00	127.75
	2826	Č.	TYR A	160	-6.239	45.240	-11.471	1.00	127.75 117.93
	2827	ŏ	TYR A	160	-5.674	45.836	-10.557	1.00	117.93
	2828	N	GLU A	161	-7.184	44.335	-11.275	1.00	99.07
35	2829	CA	GLU A	161	-7.665	43.963	-9.960	1.00	99.07
	2830	CB CB	GLU A	161	-9.179	44.113	-9.945	1.00	160.66
	2831 2832	CG CD	GLU A GLU A	161 161	-9.877	43.683 44.226	-8.681	1.00	160.66
	2833	OE1	GLU A	161	-11.290 -12,117	43.690	-8.624 -7.856	1.00 1.00	160.66 160.66
40	2834	OE2	GLU A	161	-11.564	45.206	-9.350	1.00	160.66
	2835	С	GLU A	161	-7.258	42.507	-9.699	1.00	99.07
	2836	0	GLU A	161	-7.346	41.672	-10.598	1.00	99.07
	2837	N	SER A	162	-6.806	42,206	-8.481	1.00	84.68
45	2838 2839	CA CB	SER A	162	-6.378	40.856	-8.119	1.00	84.68
40	2840	OG	SER A SER A	162 162	-5.247 -5.670	40.923 41.599	-7.102 -5.932	1.00	134.29
	2841	č	SER A	162	-7.520	40.029	-5.932 -7.536	1.00 1.00	134.29 84.68
	2842	ŏ	SER A	162	-8.592	40.555	-7.230	1.00	84.68
~ 0	2843	N	GLU A	163	-7.292	38.729	-7.382	1.00	56.84
50	2844	CA	GLU A	163	-8.316	37.829	-6.842	1.00	56.84
	2845	CB	GLU A	163	-7.885	36.370	-7.015	1.00	162.97
	2846 2847	CG CD	GLU A	163	-7.984	35.836	-8.438	1.00	162.97
	2848	OE1	GLU A GLU A	163 163	-9.417 -10.122	35.601 34.835	-8.869 -9.475	1.00	162.97
55	2849	OE2	GLU A	163	-9.835	36.176	-8.175 -9.900	1.00 1.00	162.97 162.97
	2850	C	GLU A	163	-8.437	38.151	-5.368	1.00	56.84
	2851	0	GLU A	163	-7.439	38.433	-4.720	1.00	56.84
	2852	N	PRO A	164	-9.660	38.122	-4.805	1.00	48.99
60	2853	CD	PRO A	164	-10.959	37.760	-5.379	1.00	93.04
oo	2854 2855	CA CB	PRO A	164	-9.789	38.423	-3.371	1.00	48.99
	2856	CG	PRO A PRO A	164 164	-11.295 -11.814	38.547 37.544	-3.196 -4.135	1.00	93.04
	2857	č	PRO A	164	-9.201	37.3 44 37.307	-4.135 -2.528	1.00 1.00	93.04 48.99
	2858	ŏ	PRO A	164	-9.101	36.160	-2.977	1.00	48.99
65	2859	N	LEU A	165	-8.802	37.625	-1.303	1.00	69.69
	2860	· CA	LEU A	165	-8.236	36.609	-0.426	1.00	69.69
	2861	CB	LEU A	165	-6.733	36.661	-0.465	1.00	37.26
	2862	CG CD1	LEU A	165	-6.041	35.774	0.560	1.00	37.26
70	2863 2864	CD1 CD2	LEU A LEU A	165 165	-6.655 -4.535	34.407 35.665	0.459	1.00	37.26
	2007	JU2	LEU A	100	71.333	35.665	0.301	1.00	37.26

	2005	•	1511 4	405					
	2865 2866	CO	LEU A	165 165	-8.661 -8.430	36.800 37.863	1.000 1.562	1.00	69.69
	2867	Ň	ASN A	166	-9.272	35.777	1.585	1.00 1.00	69.69
_	2868	CA	ASN A	166	-9.725	35.861	2.962	1.00	67.70 67.70
5	2869	CB	ASN A	166	-10.806	34.849	3.224	1.00	76.12
	2870 2871	CG OD1	ASN A	166	-12.182	35.396	2.998	1.00	76.12
	2872	ND2	ASN A ASN A	166 166	-12.414 -13.106	36.571 34.519	3.171 2.633	1.00	76.12
	2873	C	ASN A	166	-8.606	35.605	3.943	1.00 1.00	76.12
10	2874	0	ASN A	166	-7.724	34.792	3.687	1.00	67.70 67.70
	2875	N	ILE A	167	-8.665	36.273	5.090	1.00	54.98
	2876 2877	CA CB	ILE A	167	-7.634	36.127	6.105	1.00	54.98
	2878	CG2	ILE A	167 167	-6.686 -5.883	37.292 37.357	6.049	1.00	41.48
15	2879	CG1	ILE A	167	-5. 77 0	37.131	7.277 4.855	1.00 1.00	41.48 41.48
	2880	CD1	ILE A	167	-4.655	38.164	4.815	1.00	41.48
	2881	C	ILE A	167	-8.248	36.093	7.478	1.00	54.98
	2882 2883	0 N	ILE A THR A	167	-9.113	36.914	7.783	1.00	54.98
20	2884	CA	THR A	168 168	-7.820 -8.391	35.163 35.122	8.317	1.00	55.70
	2885	CB	THR A	168	-9.241	33.875	9.642 9.837	1.00 1.00	55.70 71.33
	2886	OG1	THR A	168	-10.289	33.866	8.860	1.00	71.33
	2887	CG2	THR A	168	-9.857	33.869	11.209	1.00	71.33
25	2888	C	THR A	168	-7.339	35.171	10.697	1.00	55.70
25	2889 2890	O N	THR A VAL A	168 169	-6.295 -7.618	34.539	10.587	1.00	55.70
	2891	CA	VAL A	169	-6. 72 5	35.950 36.090	11.724 12.863	1.00 1.00	64.35
	2892	СВ	VAL A	169	-6.370	37.560	13.087	1.00	64.35 77.36
20	2893	CG1	VAL A	169	-5.895	37.772	14.468	1.00	77.36
30	2894	CG2	VAL A	169	-5.314	37.978	12.128	1.00	77.36
	2895 2896	C	VAL A VAL A	169 169	-7.539 -8.510	35.567	14.048	1.00	64.35
	2897	Ň	ILE A	170	-7.175	36.203 34.395	14.463 14.562	1.00 1.00	64.35 76.83
	2898	CA	ILE A	170	-7.889	33.797	15.690	1.00	76.83
35	2899	СВ	ILE A	170	-7.898	32.250	15.590	1.00	133.66
	2900	CG2	ILE A	170	-8.437	31.821	14.237	1.00	133.66
	2901 2902	CG1 CD1	ILE A ILE A	170 170	-6.482	31.697	15.761	1.00	133.66
	2903	C	ILE A	170	-6.386 -7.196	30.180 34.228	15.647 16.976	1.00 1.00	133.66 76.83
40	2904	Ŏ	ILE A	170	-6.164	34.887	16.922	1.00	76.83
	2905	N	LYS A	171	-7.757	33.870	18.127	1.00	125.94
	2906	CA	LYS A	171	-7.152	34.252	19.397	1.00	125.94
	2907 2908	CB CG	LYS A LYS A	171 171	-8.004	35.328	20.069	1.00	198.00
45	2909	CD	LYS A	171	-9.449 -10.354	34.922 36.141	20.293 20.399	1.00 1.00	198.00 198.00
	2910	CE	LYS A	171	-9.952	37.059	21.546	1.00	198.00
	2911	NZ	LYS A	171	-10.825	38.268	21.607	1.00	198.00
	2912	C	LYS A	171	-6.957	33.072	20.338	1.00	125.94
50	2913 2914	O C1	LYS A NAG A	171 221	-6.326	33.204	21.388	1.00	125.94
50	2915	C2	NAG A	221	13.561 13.758	29.146 30.631	-11.328 -11.596	1.00	244.51
	2916	N2	NAG A	221	12.475	31.303	-11.575	1.00 1.00	244.51 244.51
	2917	C7	NAG A	221	12.407	32.594	-11.273	1.00	244.51
55	2918	07	NAG A	221	13.396	33.270	-10.988	1.00	244.51
22	2919	C8	NAG A	221	11.023	33.233	-11.281	1.00	244.51
	2920 2921	C3 O3	NAG A NAG A	221 221	14.405 14.740	30.847 32.219	-12.952	1.00	244.51
	2922	Č4	NAG A	221	15.661	29.997	-13.099 -13.135	1.00 1.00	244.51 244.51
~	2923	O4	NAG A	221	16.044	30.091	-14.520	1.00	244.51
60	2924	C5	NAG A	221	15.375	28.530	-12.759	1.00	244.51
	2925 2926	O5 C6	NAG A	221	14.809	28.456	-11.436	1.00	244.51
	2927	O6	NAG A NAG A	221 221	16.622	27.665	-12.740	1.00	244.51
	2928	C1	NAG A	222	17.566 17.330	28.140 29.723	-11.790 -14.890	1.00 1.00	244.51 195.02
65	2929	C2	NAG A	222	17.910	30.770	-15.864	1.00	195.02
	2930	N2	NAG A	222	17.966	32.078	-15.229	1.00	195.02
	2931	C7 .	NAG A	222	19.134	32.692	-15.052	1.00	195.02
	2932 2933	O7 C8	NAG A NAG A	222 222	20.210	32.206	·15.404	1.00	195.02
70	2934	C3	NAG A NAG A	222	19.106 17.061	34.055 30.835	-14.383 -17.148	1.00	195.02
. •		-	147W A		11.001	30.033	-17.148	1.00	195.02

	2935	03	NIAC A	***	47.004	04 675	40.400		
	2936	33 24	NAG A		17.694	31.675	-18.105	1.00	195.02°
	2937	⊙ 4	NAG A NAG A		16.869	29.431	-17.744	1.00	195.02
	2938	C5	NAG A		15.938 16.356	29.494	-18.814	1.00	195.02
5	2939	05	NAG A		17.249	28.454 28.441	-16.676	1.00	195.02
,	2940	C6	NAG A		16.248	27,029	-15.538	1.00	195.02
	2941	06	NAG A		15.013	26.448	-17.174 -16.789	1.00	195.02
	2942	C1	NAG A		-3.473	17.670	-6.472	1.00	195.02
	2943	C2	NAG A		-3.080	17.582	-7.921	1.00 1.00	81.55
10	2944	N2	NAG A		-1.712	17.148	-8.025	1.00	81.55
	2945	C7	NAG A		-1.420	16.075	-8.748	1.00	81.55
	2946	07	NAG A		-2.270	15.414	-9.324	1.00	81.55 81.55
	2947	C8	NAG A		0.033	15.657	-8.846	1.00	81.55
	2948	C3	NAG A		-3.225	18.933	-8.583	1.00	81.55
15	2949	O3	NAG A	242	-2.918	18.814	-9.969	1.00	81.55
	2950	C4	NAG A	242	-4.642	19.456	-8.403	1.00	81.55
	2951	04	NAG A	242	-4.712	20.825	-8.846	1.00	81.55
	2952	C5	NAG A	242	-5.062	19.392	-6.945	1.00	81.55
00	2953	O5	NAG A		-4.830	18.086	-6.394	1.00	81.55
20	2954	C6	NAG A		-6.547	19.630	-6.824	1.00	81.55
	2955	O 6	NAG A	-	-6.826	20.697	-5.933	1.00	81.55
	2956	C1	NAG A		-5.536	21.071	-9.934	1.00	123.88
	2957	C2	NAG A		-6.020	22.528	-9.929	1.00	123.88
25	2958	N2	NAG A		-6.814	22.800	-8.743	1.00	123.88
43	2959 2960	C7	NAG A		-6.607	23.908	-8.041	1.00	123.88
		O7	NAG A		-5.746	24.727	-8.337	1.00	123.88
	2961 2962	C8 C3	NAG A		-7.482	24.135	-6.820	1.00	123.88
	2963	∝ ⊙3	NAG A		-6.875 7.076	22.766	-11.173	1.00	123.88
30	2964	C4	NAG A	243 243	-7.276	24.126	-11.231	1.00	123.88
50	2965	04	NAG A	243	-6.109 -7.002	22.379 22.470	-12.449	1.00	123.88
	2966	C5	NAG A	243	-5.608	20.937	-13.597 -12.312	1.00 1.00	123.88
	2967	O5	NAG A		-4.793	20.809	-11.132	1.00	123.88 123.88
	2968	C6	NAG A	243	-4.789	20.444	-13.485	1.00	123.88
35	2969	O6	NAG A	243	-3.560	21.141	-13.577	1.00	123.88
	2970	C1	MAN A	244	-6.640	23.134	-14.739	1.00	177.21
	2971	C2	MAN A	244	-6.289	24.639	-14.645	1.00	177.21
	2972	02	MAN A	244	-4.892	24.794	-14.586	1.00	177.21
40	2973 2974	C3	MAN A	244	-6.845	25.182	-15.998	1.00	177.21
40	2974 2975	O3 C4	MAN A	244	-6.636	26.575	-16.149	1.00	177.21
	2976	04	MAN A	244 244	-6.314	24.396	-17.244	1.00	177.21
	2977	C5	MAN A	244	-6.840 -6.779	24.954 22.928	-18.451 -17.096	1.00	177.21
	2978	O5	MAN A	244	-6.232	22.337	-17.096	1.00 1.00	177.21
45	2979	C6	MAN A	244	-6.487	22.037	-18.309	1.00	177.21 177.21
	2980	06	MAN A	244	-5.159	21.562	-18.301	1.00	177.21
	2981	C1	NAG A	250	18.849	18.682	-1.016	1.00	245.89
	2982	C2	NAG A	250	19.989	19.613	-0.566	1.00	245.89
~ ^	2983	N2	NAG A	250	20.115	19.601	0.880	1.00	245.89
50	2984	C7	NAG A	250	21.178	19.048	1.458	1.00	245.89
	2985	07	NAG A	250	22.091	18.518	0.819	1.00	245.89
	2986	C8	NAG A	250	21.237	19.081	2.980	1.00	245.89
	2987	C3	NAG A	250	19.696	21.039	-1.050	1.00	245.89
55	2988	03	NAG A	250	20.782	21.896	-0.728	1.00	245.89
55	2989 2990	. C4 · O4	NAG A	250	19.457	21.047	-2.564	1.00	245.89
	2991	∵ O4 C5	NAG A		19.058	22.347	-2.977	1.00	245.89
	2992	O5	NAG A	250 250	18.367 18.721	20.028	-2.935	1.00	245.89
	2993	C6	NAG A	250	18.165	18.715 19.903	-2.444	1.00	245.89
60	2994	06	NAG A		17.400	18.748	-4.436 -4.760	1.00	245.89
	2995	C1	NAG A	274	2.176	9.666	16.692	1.00	245.89
	2996	C2	NAG A	274	1.514	10.512	17.789	1.00 1.00	235.37 235.37
	2997	N2	NAG A		2.519	11.269	18.514	1.00	235.37 235.37
	2998	C7	NAG A	274	2.186	12.397	19.137	1.00	235.37
65	2999	07	NAG A		1.042	12.855	19.128	1.00	235.37
	3000	C8	NAG A	274	3.289	13,134	19.882	1.00	235.37
	3001	ca	NAG A		0.750	9.604	18.761	1.00	235.37
	3002	03	NAG A		0.023	10.398	19.687	1.00	235.37
70	3003	C4	NAG A		-0.216	8.687	18.005	1.00	235.37
70	3004	04	NAG A	274	-0.794	7.758	18.909	1.00	235.37

	3005	C5	NAG A	274	0.524	7.004	40.000		
	3006	O5	NAG A	274 274	0.534 1.187	7.934 8.871	16.900 16.018	1.00 1.00	235.37
	3007	C6	NAG A	274	-0.384	7.085	16.044	1.00	235.37 235.37
	3008	O6	NAG A	274	0.294	6.598	14.895	1.00	235.37
5	3009	C1	NAG A	33 5	7.685	42.617	-1.591	1.00	248.30
	3010	C2	NAG A	335	8.870	42.060	-0.765	1.00	248.30
	3011	N2	NAG A	335	8.767	42.587	0.583	1.00	248.30
	3012 3013	C7 O7	NAG A NAG A	335 335	8.573 8.483	41.777	1.618	1.00	248.30
10	3014	C8	NAG A	335	8.472	40.553 42.430	1.511 2.987	1.00 1.00	248.30
	3015	C3	NAG A	335	10.258	42.417	-1.325	1.00	248.30 248.30
	3016	O3	NAG A	335	11.229	41.541	-0.771	1.00	248.30
	3017	C4	NAG A	335	10.290	42.300	-2.841	1.00	248.30
15	3018	04	NAG A	335	11.560	42.706	-3.329	1.00	248.30
13	3019 3020	C5 O5	NAG A NAG A	335 335	9.195	43.189	-3.414	1.00	248.30
	3020	C6	NAG A	335 335	7.904 9.222	42.673 43.210	-3.021 -4.935	1.00	248.30
	3022	06	NAG A	335	9.423	44.524	-5.434	1.00 1.00	248.30 248.30
	3023	C1	NAG A	340	0.521	43.731	20.574	1.00	249.48
20	3024	C2	NAG A	340	-0.261	42.929	21.588	1.00	249.48
	3025	N2	NAG A	340	-1.284	42.144	20.930	1.00	249.48
	3026	C7	NAG A	340	-1.377	40.843	21.191	1.00	249.48
	3027 3028	O7 C8	NAG A NAG A	340 340	-0.627 -2.460	40.266	21.988	1.00	249.48
25	3029	ČŠ	NAG A	340	-0.877	40.060 43.866	20.472 22.605	1.00 1.00	249.48
;	3030	03	NAG A	340	-1.567	43.103	23.596	1.00	249.48 249.48
	3031	C4	NAG A	340	0.234	44.689	23.266	1.00	249.48
	3032	04	NAG A	340	-0.370	45.703	24.068	1.00	249.48
30	3033	C5	NAG A	340	1.188	45.334	22.220	1.00	249.48
30	3034 3035	O5 C6	NAG A NAG A	340 340	1.601	44.382	21.233	1.00	249.48
	3036	06	NAG A	340	2.460 3.548	45.780 45.816	22.881 21.985	1.00 1.00	249.48
	3037	C1	NAG A	366	-14.447	34.952	2.337	1.00	249.48 170.79
~~	3038	C2	NAG A	366	-15.009	34.055	1.250	1.00	170.79
35	3039	N2	NAG A	366	-14.171	34.149	0.073	1.00	170.79
	3040	C7	NAG A	366	-13.171	33.289	-0.105	1.00	170.79
	3041 3042	07 C8	NAG A NAG A	366 366	-12.912	32.383	0.691	1.00	170.79
	3043	C3	NAG A	366	-12.329 -16.425	33.454 34.482	-1.361 0.910	1.00 1.00	170.79
40	3044	03	NAG A	366	-16.997	33.542	0.014	1.00	170.79 170.79
	3045	C4	A DAN	366	-17.290	34.565	2.168	1.00	170.79
	3046	04	NAG A	366	-18.549	35.187	1.824	1.00	170.79
	3047 3048	C5	NAG A	366	-16.584	35.380	3.275	1.00	170.79
45	3048	O5 C6	NAG A NAG A	366 366	-15.258 -17.297	34.873	3.503	1.00	170.79
	3050	06	NAG A	366	-16.620	35.315 36.092	4.613 5.592	1.00 1.00	170.79
	3051	C1	NAG A	367	-19.711	34.493	2,163	1.00	170.79 247.02
	3052	C2	NAG A	367	-20.892	35.462	2.268	1.00	247.02
50	3053	N2	NAG A	367	-20.619	36.488	3.255	1.00	247.02
20	3054 3055	C7 O7	NAG A	367	-20.363	37.730	2.856	1.00	247.02
	3056	C8	NAG A NAG A	367 367	-20.347	38.061	1.668	1.00	247.02
	3057	ä	NAG A	367	-20.084 -22.151	38.762 34.676	3.937 2.640	1.00 1.00	247.02
	3058	03	NAG A	367	-23.265	35.554	2.696	1.00	247.02 247.02
55	3059	C4	NAG A	367	-22.395	33.586	1.591	1.00	247.02
	3060	04	NAG A	367	-23 511	32.793	1.970	1.00	247.02
	3061 3062	C5 OF	NAG A	367	-21.148	32.698	1.448	1.00	247.02
	3063	O5 C6	NAG A NAG A	367 367	-19.981 -21. 2 91	33.508	1.147	1.00	247.02
60	3064	06	NAG A	367	-20.416	31.682 31.974	0.332 -0.749	1.00 1.00	247.02
	3065	CB	LYS B	4	28.538	57.342	22.861	1.00	247.02 248.35
	3066	CG	LYS B	4	28.723	58.799	22.474	1.00	248.35
	3067	CD	LYS B	4	28.723	59.692	23.702	1.00	248.35
65	3068	CE	LYS B	4	28.914	61.151	23.330	1.00	248.35
0 5	3069 3070	NZ C	LYS B	4	28.914	62.022	24.537	1.00	248.35
	3071	ŏ	LYS B	4	29.934 30.913	56.599 57.081	20.941	1.00	249.33
	3072	Ň	LYS B	4	28.491	54.970	21.514 22.165	1.00 1.00	249.33 249.33
70	3073	CA	LYS B	4	28.619	56.377	21.683	1.00	249.33
70	3074	N	PRO B	5	29.974	56.244	19.648	1.00	115.49

	3075	CD	PRO B	5 -	28.994	55.392	18.958	1.00	70.51
	3076	CA	PRO B		31.186	56.414	18.835	1.00	115.49
	3077	CB	PRO B		31.037	55.337	17.765	1.00	70.51
5	3078	CG	PRO B		29.573	55.299	17.553	1.00	70.51
3	3079 3080	C	PRO B		31.329	57.807	18.247	1.00	115.49
	3081	N	LYS B		30.350 32.553	58.537 58.174	18.126	1.00	115.49
	3082	CA	LYS B		32.553	59.492	17.885 17.331	1.00	105.72
	3083	CB	LYS B		33.258	60.458	18.449	1.00 1.00	105.72
10	3084	CG	LYS B		33.432	61.901	17.991	1.00	206.94 206.94
	3085	CD	LYS B		33.697	62.850	19.152	1.00	206.94
	3086	CE	LYS B		33.826	64.287	18.654	1.00	206.94
	3087 3088	NZ C	LYS B	_	34.006	65.275	19.759	1.00	206.94
15	3089	ŏ	LYS B	6 6	33.857 35.018	59.429 59.109	16.222	1.00	105.72
	3090	Ň	VAL B	7	33.433	59.742	16.467 15.002	1.00	105.72
	3091	CA	VAL B	7	34.317	59.728	13.843	1.00 1.00	68.17 68.17
	3092	CB	VAL B	7	33.553	59.960	12.545	1.00	86.47
20	3093	CG1	VAL B	7	34.487	59.738	11.359	1.00	86.47
20	3094	CG2	VAL B	7	32.346	59.072	12.479	1.00	86.47
	3095 3096	C O	VAL B	7	35.401	60.796	13.845	1.00	68.17
	3097	N .	. VAL B SER B	7 8	35.094 36.661	61.988 60.385	13.803	1.00	68.17
	3098	ĊA	SER B	8	37.741	61.355	13.864 13.837	1.00 1.00	61.68
25	3099	СВ	SER B	8	38.836	60.969	14.842	1.00	61.68 135.50
	3100	OG	SER B	8	39.289	59.647	14.622	1.00	135.50
	3101	C	SER B	8	38.303	61.405	12.406	1.00	61.68
	3102 3103	0	SER B	8	38.019	60.525	11.594	1.00	61.68
30	3103	N CA	LEU B	9 9	39.092 39.699	62.435	12.106	1.00	91.60
50	3105	CB	LEU B	9	39.080	62.594 63.779	10.790 10.053	1.00	91.60
	3106	CG	LEU B	9	37.601	63.806	9.688	1.00 1.00	67.13
	3107	CD1	LEU B	9	37.378	64.735	8.524	1.00	67.13 67.13
25	3108	CD2	LEU B	9	37.167	62.435	9.291	1.00	67.13
35	3109	C	LEU B	9	41.195	62.847	10.897	1.00	91.60
	3110 3111	0 N	LEU B ASN B	9	41.675	63.347	11.915	1.00	91.60
	3112	ČA	ASN B	10 10	41.928 43.369	62.519 62.742	9.835 9.800	1.00	84.59
	3113	CB	ASN B	10	44.107	61.640	10.548	1.00 1.00	84.59 140.61
40	3114	CG	ASN B	10	45.558	61.978	10.763	1.00	140.61
	3115	OD1	ASN B	10	45.889	62.905	11.505	1.00	140.61
	3116	ND2	ASN B	10	46.438	61.241	10.099	1.00	140.61
	3117 3118	C	ASN B	10	43.876	62.812	8.367	1.00	84.59
45	3119	Ň	PRO B	10 11	43.883 44.310	61.805 64.010	7.656	1.00	84.59
	3120	ČD	PRO B	11	44.699	64.185	7.917 6.506	1.00 1.00	77.61
	3121	CA	PRO B	11	44.370	65.289	8.638	1.00	115.85 77.61
	3122	CB	PRO B	11	44.811	66.264	7.544	1.00	115.85
50	3123	CG	PRO B	11	45.560	65.394	6.570	1.00	115.85
30	3124 3125	C	PRO B	11	43.042	65.731	9.290	1.00	77.61
	3125	Ň	PRO B	11	41.982	65.231	8.937	1.00	77.61
	3127	ČD	PRO B	12 12	43.085 44.279	66.680 67.378	10.239	1.00	88.06
	3128	CA	PRO B	12	41.883	67.170	10.753 10. 921	1.00 1.00	174.82 88.06
55	3129	CB	PRO B	12	42.433	68.119	11.982	1.00	174.82
	3130	CG	PRO B	12	43.854	67.699	12.148	1.00	174.82
	3131	C	PRO B	12	40.993	67.939	9.924	1.00	88.06
	3132 3133	O N	PRO B	12	39.781	68.071	10.108	1.00	88.06
60	3134	ĞA	TRP B	13 13	41.623 40.932	68.464	8.880	1.00	96.43
	3135	CB	TRP B	13	41.907	69.239 69.605	7.859 6.731	1.00	96.43
	3136	CG	TRP B	13	43.190	70.134	7.232	1.00 1.00	96.49 96.49
	3137	CD2	TRP B	13	43.376	70.974	8.358	1.00	96.49
65	3138	CE2	TRP B	13	44.757	71.168	8.509	1.00	96.49
U)	3139	CE3	TRP B	13	42.504	71.588	9.268	1.00	96.49
	3140 3141	CD1 NE1	TRP B	13	44.423	69.863	6.745	1.00	96.49
	3142	CZ2	TRP B	13 13	45.373 45.298	70.474 71.047	7.506	1.00	96.49
	3143	CZ3	TRP B	13	43.034	71.947 72.363	9.532 10.283	1.00 1.00	96.49
70	3144	CH2	TRP B	13	44.424	72.536	10.410	1.00	96.49 96.49
									80.73

	3145	Ç	TRP B	13	39.742	68.497	7.281	1.00	96.43
	3146	0	TRP B	13	39.882	67.403	6.738	1.00	96.43
	3147	N	ASN B	14	38.567	69.102	7.407	1.00	72.14
_	3148	CA	ASN B	14	37.352	68.509	6.867	1.00	72.14
5	3149	CB	ASN B	14	36.239	68.455	7.931	1.00	117.87
	3150	CG	ASN B	14	35.712	69.812	8.309	1.00	
	3151	OD1	ASN B	14	36.462	70.695	8.718	1.00	117.87
	3152	ND2	ASN B	14	34.407	69.984	8.184	1.00	117.87
	3153	С	ASN B	14	36.858	69.201	5.588	1.00	117.87
10	3154	0	ASN B	14	35.721	69.018	5.177	1.00	72.14
	3155	N	ARG B	15	37.715	70.009	4.973		72.14
	3156	CA	ARG B	15	37.399	70.653	3.701	1.00	61.00
	3157	СВ	ARG B	15	37.241	72.149	3.841	1.00	61.00
	3158	ČĞ	ARG B	15	36.513	72.149 72.569		1.00	68.74
15	3159	CD	ARG B	15	36.354		5.064	1.00	68.74
	3160	NE	ARG B	15	35.436	74.075	5.045	1.00	68.74
	3161	CZ	ARG B	15		74.525	4.007	1.00	68.74
	3162	NH1	ARG B		35.531	75.714	3.429	1.00	68.74
	3163	NH2	ARG B	15	36.501	76.533	3.794	1.00	68.74
20	3164	C	ARG B	15	34.660	76.093	2.498	1.00	68.74
20	3165	ŏ	ARG B	15	38.662	70.393	2.900	1.00	61.00
	3166	Ň		15	39.707	70.950	3.199	1.00	61.00
	3167	CA		16	38.587	69.540	1.895	1.00	73.69
		CB	ILE B	16	39.770	69.256	1.135	1.00	73.69
25	3168		ILE B	16	40.194	67.833	1.339	1.00	63.86
23	3169	CG2	ILE B	16	40,624	67.645	2.767	1.00	63.86
	3170	CG1	ILE B	16	39.044	66.895	0.994	1.00	63.86
	3171	CD1	ILE B	16	39.388	65.448	1.178	1.00	63.86
	3172	C	ILE B	16	39.621	69.493	-0.340	1.00	73.69
30	3173	0	ILE B	16	38.516	69.651	-0.866	1.00	73.69
30	3174	N	PHE B	17	40.770	69.491	-0.998	1.00	99.56
	3175	CA	PHE B	17	40.889	69.696	-2.425	1.00	99.56
	3176	CB	PHE B	17	42.282	70.211	-2.720	1.00	81.03
	3177	CG	PHE B	17	42.400	71.703	-2.699	1.00	81.03
35	3178	CD1	PHE B	17	43.515	72.315	-2.128	1.00	81.03
33	3179	CD2	PHE B	17	41.453	72.497	-3.344	1.00	81.03
	3180	CE1	PHE B	17	43.685	73.688	-2.204	1.00	81.03
	3181	CE2	PHE B	17	41.613	73.877	-3.428	1.00	81.03
	3182	CZ	PHE B	17	42.733	74.475	-2.860	1.00	81.03
40	3183	C	PHE B	17	40.678	68.392	-3.169	1.00	99.56
40	3184	0	PHE B	17	40.804	67.321	-2.591	1.00	99.56
	3185	N	LYS B	18	40.374	68.484	-4.459	1.00	100.47
	3186	CA	LYS B	18	40.160	67.302	-5.288	1.00	100.47
	3187	CB	LYS B	18	39.700	67.733	-6.682	1.00	201.96
45	3188	CG	LYS B	18	39.302	66.601	-7.612	1.00	201.96
43	3189	CD	LYS B	18	38.552	67.166	-8.809	1.00	201.96
	3190	CE	LYS B	18	38.122	66.086	-9.776	1.00	201.96
	3191	NZ	LYS B	18	39.299	65.382	-10.345	1.00	201.96
	3192	C	LYS B	18	41.448	66.492	-5.394	1.00	100.47
50	3193	0	LYS B	18	42.518	67.028	-5. 67 1	1.00	100.47
50	3194	N	GLY B	19	41.362	65.197	-5.143	1.00	85.25
	3195	CA	GLY B	19	42.547	64.371	-5.264	1.00	85.25
	3196	С	GLY B	19	43.350	64.115	-4.008	1.00	85.25
	3197	O	GLY B	19	44.237	63.274	-3.996	1.00	85.25
F F	3198	N	GLU B	20	43.057	64.825	-2.937	1.00	70.09
55	3199	CA	GLU B	20	43.804	64.606	-1.701	1.00	70.09
	3200	CB	GLU B	20	43.005	65.846	-0.813	1.00	167.13
	3201	CG	GLU B	20	44.020	67.133	-1.566	1.00	167.13
	3202	CD	GLU B	20	44.034	68.357	-0.677	1.00	167.13
	3203	OE1	GLU B	20	43.009	68.622	-0.013	1.00	167.13
60	3204	OE2	GLU B	20	45.070	69.056	-0.655	1.00	167.13
	3205	С	GLU B	20	43.296	63.356	-0.967	1.00	
	3206	0	GLU B	20	42.273	62.769	-1.368	1.00	70.09
	3207	N	ASN B	21	44.002	62.935	0.086	1.00	70.09 77.36
	3208	CA	ASN B	21	43.579	61.747	0.830		
65	3209	CB	ASN B	21	44.626	60.630	0.802	1.00	77.36
	3210	CG	ASN B	21	45.285	60.472	-0.537	1.00	155.50
	3211	OD1	ASN B	21	44.634	60.520	-0.537 -1.585	1.00	155.50
	3212	ND2	ASN B	21	46.598	60.265	-1.585 -0.490	1.00	155.50
	3213	C	ASN B	21	43.300	62.066	2.287	1.00	155.50
70	3214	Ŏ	ASN B	21	43.997	62.877	2.892	1.00	77.36
						V//	2.002	1.00	77.36

	3215	N	VAL B	22	42.286	61.409	2.848	1.00	68.07
	3216	CA	VAL B	22	41.899	61.602	4.241	1.00	68.07
	3217 3218	CB CG1	VAL B VAL B	22	40.732	62,572	4.364	1.00	74.66
5	3219	CG2	VAL B	22 22	39.514	62.023	3.658	1.00	74.66
•	3220	C	VAL B	22	40.438 41.469	62.807 60.270	5.811	1.00	74.66
	3221	ŏ	VAL B	22	40.964	59.391	4.829 4.120	1.00	68.07
	3222	N	THR B	23	41.646	60.123	6.132	1.00 1.00	68.07
	3223	CA	THR B	23	41.316	58.865	6.791	1.00	73.02
10	3224	CB	THR B	23	42.576	58.274	7.428	1.00	73.02 107.36
	3225	OG1	THR B	23	43.602	58.155	6.435	1.00	107.36
	3226 3227	CG2	THR B	23	42.288	56.919	8.018	1.00	107.36
	3228	c o	THR B	23	40.278	59.057	7.885	1.00	73.02
15	3229	N	LEU B	23 24	40.446	59.918	8.739	1.00	73.02
	3230	CA	LEU B	24 24	39.211 38.180	58.261 58.423	7.888	1.00	82.14
	3231	CB	LEU B	24	36.771	58.497	8.920 8.323	1.00	82.14
	3232	CG	LEU B	24	36.534	59.233	6.996	1.00 1.00	67.63
20	3233	CD1	LEU B	24	35.063	59.448	6.787	1.00	67.63 67.63
20	3234	CD2	LEU B	24	37.249	60.554	6.987	1.00	67.63
	3235	C	LEU B	24	38.205	57.286	9.904	1.00	82.14
	3236 3237	0 N	LEU B	24	37.732	56.195	9.615	1.00	82.14
	3238	CA	THR B THR B	25	38.735	57.551	11.086	1.00	78.19
25	3239	CB	THR B	25 25	38.817 ::2.047	56.519	12.099	1.00	78.19
	3240	OG1	THR B	25	41.200	56.755 56.846	12.971	1.00	154.05
	3241	CG2	THR B	25	40.231	55.618	12.124 13.949	1.00 1.00	154.05
	3242	C	THR B	25	37.554	56.489	12.941	1.00	154.05 78.19
20	3243	0	THR B	25	37.022	57.532	13.310	1.00	78.19 78.19
30	3244	N	CYS B	26	37.044	55.296	13.210	1.00	82.94
	3245 3246	CA	CYS B	26	35.860	55.184	14.049	1.00	82.94
	3247	C O	CYS B CYS B	26	36.280	55.187	15.510	1.00	82.94
	3248	СВ	CYS B	26 26	37.254 35.094	54.549	15.896	1.00	82.94
35	3249	SG	CYS B	26	33.481	53.908 53.869	13.763	1.00	125.46
	3250	N	ASN B	27	35.535	55.931	14.604 16.309	1.00 1.00	125.46
	3251	CA	ASN B	27	35.784	56.058	17.730	1.00	247.26 247.26
	3252	CB	ASN B	27	34.500	55.740	18.470	1.00	240.69
40	3253 3254	CG	ASN B	27	34.506	56.280	19.864	1.00	240.69
40	3254 3255	OD1	ASN B	27	35.033	57.371	20.107	1.00	240.69
	3256	ND2 C	ASN B ASN B	27	33.909	55.541	20.797	1.00	240.69
	3257	ŏ	ASN B	27 27	36.922 36.702	55.201 54.072	18.289	1.00	247.26
	3258	Ň	GLY B	28	38.135	55.748	18.722 18.286	1.00	247.26
45	3259	CA	GLY B	28	39.286	55.021	18.792	1.00 1.00	195.90 195.90
	3260	С	GLY B	28	40.518	55.841	18.506	1.00	195.90
	3261	· · O	GLY B	28	40.788	56.161	17.355	1.00	195.90
	3262	N	ASN B	29	41.274	56.181	19.541	1.00	230.48
50	3263 3264	CA CB	ASN B	29	42.456	57.003	19.352	1.00	230.48
20	3265	CG	ASN B ASN B	29 29	42.882 43.919	57.612	20.690	1.00	249.51
	3266	OD1	ASN B	29	44.154	58.710 59.198	20.527	1.00	249.51
	3267	ND2	ASN B	29	44.534	59.196 59.115	19.421	1.00	249.51
	3268	C	ASN B	29	43.644	56.302	21.634 18.699	1.00 1.00	249.51
55	3269	0	ASN B	29	44.198	56.804	17.716	1.00	230.48 230.48
	3270	N	ASN B	30	44.040	55.149	19.229	1.00	218.47
	3271	CA	ASN B	30	45.185	54.441	18.667	1.00	218.47
	3272 3273	CB	ASN B	30	46.364	54.509	19.631	1.00	238.45
60	3274	CG OD1	ASN B ASN B	30	46.841	55.909	19.854	1.00	238.45
••	3275	ND2	ASN B	30 30	46.936 47.139	56.337	20.986	1.00	238.45
	3276	C	ASN B	30	44.936	56.635 52.990	18.778	1.00	238.45
	3277	0	ASN B	30	44.881	52.646	18.293 17.109	1.00	218.47
	3278	N	PHE B	31	44.779	52.137	19.300	1.00 1.00	218.47 249.37
65	3279	CA	PHE B	31	44.573	50.724	19.037	1.00	249.37 249.37
	3280	CB	PHE B	31	45.620	49.901	19.799	1.00	234.42
	3281 3282	CG	PHE B	31	47.045	50.311	19.513	1.00	234.42
	3282	CD1 CD2	PHE B	31	47.600	51.429	20.131	1.00	234.42
70	3284	CE1	PHE B PHE B	31 31	47.822	49.594	18.607	1.00	234.42
				JI .	48.909	51.828	19.854	1.00	234.42

	3285	CE2	PHE B	31-	49.131	49.985	18.322	1.00	234.42
	3286 3287	CZ C	PHE B	31	49.674	51.107	18.947	1.00	234.42
	3288	Ö	PHE B PHE B	31 31	43.166	50.221	19.340	1.00	249.37
5	3289	Ň	PHE B	32	42.638 42.579	50.399 49.581	20.440	1.00	249.37
_	3290	CA	PHE B	32	41.233	49.034	18. 332 18.408	1.00 1.00	162.47
	3291	СВ	PHE B	32	40.337	49.732	17.386	1.00	162.47 249.69
	3292	CG	PHE B	32	38.872	49.480	17.598	1.00	249.69
10	3293	CD1	PHE B	32	38.241	49.969	18.718	1.00	249.69
10	3294 3295	CD2	PHE B	32	38.130	48.733	16.690	1.00	249.69
	3295 3296	CE1 CE2	PHE B	32	36.894	49.721	18.931	1.00	249.69
	3297	CZ	PHE B PHE B	32 32	36.772 36.170	48.482	16.901	1.00	249.69
	3298	C	PHE B	32	41.243	48.988 47.533	18.039 18.118	1.00	249.69
15	3299	ō	PHE B	32	42.275	46.987	17.714	1.00 1.00	162.47
	3300	N	GLU B	33	40.097	46.869	18.298	1.00	162.47 249.28
	3301	CA	GLU B	33	40.035	45.425	18.046	1.00	249.28
	3302	CB	GLU B	33	39.767	44.643	19.298	1.00	249.25
20	3303 3304	CG CD	GLU B	33	39.978	43.139	19.158	1.00	249.25
20	3305	OE1	GLU B GLU B	33 33	41.395	42.776	18.727	1.00	249.25
	3306	OE2	GLU B	33	42.373 41.565	43.401 41.829	19.192 17.938	1.00	249.25
	3307	c	GLU B	33	38.993	44.918	17.938	1.00 1.00	249.25
	3308	0	GLU B	33	39.312	44.164	16.171	1.00	249.28 249.28
25	3309	N	VAL B	34	37.732	45.243	17.348	1.00	234.23
	3310	CA	VAL B	34	36.657	44.756	16.507	1.00	234.23
	3311	CB	VAL B	34	35.301	45.388	16.902	1.00	191.69
	3312 3313	CG1 CG2	VAL B VAL B	34	34.197	44.865	15.998	1.00	191.69
30	3314	C	VAL B	34 34	34.978 36.919	45.059 44.972	18.343	1.00	191.69
	3315	ŏ	VAL B	34	37.592	45.923	15.029 14.632	1.00 1.00	234.23
	3316	N	SER B	35	36.395	44.052	14.229	1.00	234.23 249.39
	3317	CA	SER B	35	36.536	44.110	12.789	1.00	249.39
35	3318	CB	SER B	35	37.053	42.775	12.246	1.00	187.29
33	3319 3320	C OG	SER B	35	36.078	41.759	12.404	1.00	187.29
	3321	ŏ	SER B SER B	35 35	35.161	44.414	12.202	1.00	249.39
	3322	Ň	SER B	36	35.008 34.160	44.523 44.541	10.988	1.00	249.39
	3323	ĊA	SER B	36	32.796	44.846	13.074 12.641	1.00 1.00	236.03 236.03
40	3324	CB	SER B	36	31.770	43.967	13.369	1.00	174.69
	3325	OG	SER B	36	31.663	44.323	14.735	1.00	174.69
	3326	Ç	SER B	36	32.488	46.310	12.911	1.00	236.03
	3327 3328	O N	SER B	36	32.037	46.684	13.992	1.00	236.03
45	3329	CA	THR B THR B	37 37	32.752	47.137	11.910	1.00	186.56
	3330	CB	THR B	37	32.516 33.852	48.565 49.349	11.996 11.926	1.00 1.00	186.56
	3331	OG1	THR B	37	34.720	48.919	12.983	1.00	204.69 204.69
	3332	CG2	THR B	37	33.611	50.838	12.065	1.00	204.69
50	3333	Ç	THR B	37	31.649	48.899	10.789	1.00	186.56
50	3334	0	THR B	37	31.837	A8.338	9.708	1.00	186.56
	3335 3336	N CA	LYS B	38	30.692	49.800	10.972	1.00	233.53
	3337	CB	LYS B LYS B	38	29.803	50.182	9.883	1.00	233.53
	3338	CG	LYS B	38 38	28.358 28.005	50.059 48.688	10.341 10.851	1.00	159.29
55	3339	CD	LYS B	38	26.556	48.633	11.299	1.00 1.00	159.29
	3340	CE	LYS B	38	26.179	47.229	11.738	1.00	159.29 159.29
	3341	NZ	LYS B	38	24.755	47.156	12.158	1.00	159.29
	3342	Č	LYS B	38	30.055	51.604	9.402	1.00	233.53
60	3343 3344	0	LYS B	38	30.349	52.490	10.203	1.00	233.53
00	3345	N CA	TRP B TRP B	39	29.936	51.818	8.092	1.00	87.42
	3346	CB	TRP B	39 39	30.140 31.422	53.149	7.521	1.00	87.42
	3347	ČĠ	TRP B	39	32.678	53.229 53.035	6.688 7.471	1.00 1.00	107.80
	3348	CD2	TRP B	39	33.240	53.923	8.438	1.00	107.80 107.80
65	3349	CE2	TRP B	39	34.427	53.326	8.904	1.00	107.80
	3350	CE3	TRP B	39	32.857	55.160	8.954	1.00	107.80
	3351	CD1	TRP B	39	33.521	51.968	7.395	1.00	107.80
	3352 3353	NE1 CZ2	TRP B	39	34.574	52.135	8.253	1.00	107.80
70	3354	CZ2	TRP B TRP B	39	35.236 33.650	53.930 55.755	9.860	1.00	107.80
	••••		IRF 0	39	33.659	55.755	9.899	1.00	107.80

	3355 3356 3357	CH2 C O	TRP B TRP B TRP B	39 39 39	34.839 28.973 28.580	55.141 53.500 52.712	10.346 6.637 5.799	1.00	107.80 87.42
	3358	Ň	PHE B	40	28.429	54.694	5.7 99 6.818	1.00 1.00	87.42
5	3359	CA	PHE B	40	27.289	55.111	6.025	1.00	127.18 127.18
	3360	CB	PHE B	40	26.052	55.264	6.908	1.00	155.57
	3361 3362	CG CD1	PHE B	40	25.605	54.032	7.687	1.00	155.57
	3363	CD1	PHE B PHE B	40 40	26.374 24.666	53.715	8.858	1.00	155.57
10	3364	CE1	PHE B	40	24.000 26.024	53.200 52.589	7.261 9.600	1.00 1.00	155.57
	3365	CE2	PHE B	40	24.308	52.074	7.991	1.00	155.57 155.57
	3366	CZ	PHE B	40	24.987	51.764	9.162	1.00	155.57
	3367	C	PHE B	40	27.523	56.414	5.281	1.00	127.18
15	3368 3369	0 N	PHE B	40	27.208	57.495	5.773	1.00	127.18
13	3370	CA	HIS B HIS B	41 41	28.078 28.329	56.306 57.484	4.084	1.00	72.05
	3371	CB	HIS B	41	29.355	57.132	3.260 2.173	1.00 1.00	72.05
	3372	CG	HIS B	41	29.650	58.256	1.230	1.00	83.13 83.13
20	3373	CD2	HIS B	41	29.801	58.274	-0.114	1.00	83.13
20	3374	ND1	HIS B	41	29.837	59.553	1.656	1.00	83.13
	3375 3376	CE1 NE2	HIS B HIS B	41 41	30.087	60.323	0.614	1.00	83.13
	3377	C	HIS B	41	30.071 27.010	59.571 57.961	-0.472 2.633	1.00	83.13
	3378	ŏ	HIS B	41	26.458	57.298	1.761	1.00 1.00	72.05 72.05
25	3379	N	ASN B	42	26.527	59.123	3.069	1.00	104.44
	3380	CA	ASN B	42	25.256	59.683	2.600	1.00	104.44
	3381	CB	ASN B	42	25.240	59.870	1.077	1.00	64.53
	3382 3383	CG OD1	ASN B ASN B	42	26.091	61.039	0.625	1.00	64.53
30	3384	ND2	ASN B	42 42	27.195 25.618	61.213	1.144	1.00	64.53
	3385	C	ASN B	42	24.114	61.828 58.751	-0.348 2.999	1.00 1.00	64.53
	3386	0	ASN B	42	23.089	58.706	2.334	1.00	104.44 104.44
	3387	N	GLY B	43	24.293	58.003	4.083	1.00	163.92
35	3388	CA	GLY B	43	23.246	57.092	4.522	1.00	163.92
33	3389 3390	C O	GLY B GLY B	43 43	23.405	55.677	3.991	1.00	163.92
	3391	Ň	SER B	43 44	23.159 23.816	54.701 55.562	4.702 2.735	1.00	163.92
	3392	CA	SER B	44	24.017	54.262	2.106	1.00 1.00	175.12 175.12
40	3393	CB	SER B	44	24.326	54.445	0.620	1.00	173.04
40	3394	og	SER B	44	23.344	55.253	-0.002	1.00	173.04
	3395 3396	C O	SER B SER B	44	25.178	53.524	2.772	1.00	175.12
	3397	Ñ	LEU B	44 45	26.275 24.944	54.070 52.285	2.899	1.00	175.12
	3398	ČA	LEU B	45	25.991	52.265 51.495	3.197 3.846	1.00 1.00	151.43
45	3399	CB	LEU B	45	25.458	50.101	4.198	1.00	151.43 163.91
	3400	CG	LEU B	45	26.424	49.160	4.922	1.00	163.91
	3401	CD1	LEU B	45	26.972	49.825	6.176	1.00	163.91
	3402 3403	CD2 C	LEU B LEU B	45	25.701	47.872	5.275	1.00	163.91
50	3404	ŏ	LEU B	45 45	27.220 27.089	51.376 51.318	2.944	1.00	151.43
	3405	Ň	SER B	46	28.411	51.350	1.722 3.541	1.00 1.00	151.43
	3406	CA	SER B	46	29.646	51.241	2.770	1.00	127.11 127.11
	3407	CB	SER B	46	30.724	52.142	3.366	1.00	226.86
55	3408	og	SER B	46	31.902	52,103	2.574	1.00	226.86
JJ	3409 3410	C	SER B SER B	46 46	30.103	49.791	2.810	1.00	127.11
	3411	Ň	GLU B	46 47	29.622 31.030	49.009	3.626	1.00	127.11
	3412	CA	GLU B	47	31.486	49.425 48.041	1.927 1.929	1.00 1.00	149.05
60	3413	СВ	GLU B	47	31.711	47.509	0.484	1.00	149.05 195.89
60	3414	CG	GLU B	47	30.777	48.077	-0.608	1.00	195.89
	3415	CD	GLU B	47	31.343	47.934	-2.030	1.00	195.89
	3416 3417	OE1 OE2	GLU B	47	32.086	48.832	-2.508	1.00	195.89
	3418	C	GLU B GLU B	47 47	31.042 32.738	46.909 47.807	-2.685	1.00	195.89
65	3419	ŏ	GLU B	47	33.224	47.807 46.684	2.808 2.891	1.00 1.00	149.05 149.05
	3420	N	GLU B	48	33.291	48.851	3.436	1.00	149.05
	3421	CA	GLU B	48	34.458	48.628	4.299	1.00	101.79
	3422	CB	GLU B	48	35.331	49.904	4.457	1.00	223.78
70	3423 3424	CG CD	GLU B	48	36.479	49.790	5.499	1.00	223.78
	J-14-4	35	GLU B	48	37.584	48.801	5.127	1.00	223.78

	3425	OE1	GLU B	48	38.340	49.074	4.170	1.00	200 70
	3426	OE2	GLU B	48	37.703	47.751	5.799	1.00	223.78
	3427	Č	GLU B	48	33.949	48.158	5.661	1.00	223.78 101.79
5	3428	0	GLU B	48	32.788	48.397	6.021	1.00	101.79
2	3429 3430	N	THR B	49	34.812	47.476	6.410	1.00	169.38
	3431	CA CB	THR B	49	34.445	46.976	7.728	1.00	169.38
	3432	OG1	THR B	49	34.268	45.441	7.707	1.00	162.45
	3433	CG2	THR B	49 49	35.467	44.824	7.222	1.00	162.45
10	3434	C	THR B	49	33.110 35.501	45.061	6.797	1.00	162.45
	3435	ŏ	THR B	49	35.190	47.369 47.530	8.762	1.00	169.38
	3436	N	ASN B	50	36.745	47.530 47.531	9.940 8.319	1.00	169.38
	3437	CA	ASN B	50	37.830	47.919	9.213	1.00 1.00	110.90
	3438	CB	ASN B	50	39.130	48.104	8.418	1.00	110.90
15	3439	CG	ASN B	50	40.355	48.183	9.311	1.00	249.40 249.40
	3440	OD1	ASN B	50	40.232	48.440	10.508	1.00	249.40
	3441	ND2	ASN B	50	41.539	47.979	8.738	1.00	249.40
	3442	Ç	ASN B	50	37.403	49.246	9.854	1.00	110,90
20	3443	0	ASN B	50	36.644	50.010	9.250	1.00	110.90
20	3444 3445	N CA	SER B	51	37.872	49.520	11.072	1.00	116.16
	3446	CB	SER B SER B	51	37.515	50.763	11.761	1.00	116.16
	3447	OG	SER B	51	38.004	50.728	13.210	1.00	152.88
	3443	c	SER B	51 51	39.421	50.782	13.277	1.00	152.88
25	3449	ŏ	SER B	51	38.084 37.632	52.007	11.066	1.00	116.16
	3450	Ñ	SER B	52	39.080	53.121 51.819	11.313	1.00	116.16
	3451	CA	SER B	52	39.684	52.939	10.206 9.501	1.00	154.44
	3452	СВ	SER B	52	41.210	52.899	9.637	1.00 1.00	154.44
20	3453	OG	SER B	52	41.611	53.078	10.987	1.00	81.31 81.31
30	3454	С	SER B	52	39.294	52.908	8.036	1.00	154.44
	3455	0	SER B	52	39.754	52.057	7.273	1.00	154.44
	3456	N	LEU B	53	38.433	53.844	7.656	1.00	115.15
	3457	CA	LEU B	53	37.961	53.963	6.280	1.00	115.15
35	3458 3459	CB	LEU B	53	36.477	54.348	6.281	1.00	65.06
55	3460	CG CD1	LEU B	53	35.882	55.021	5.036	1.00	65.06
	3461	CD2	LEU B	53 53	36.353	54.301	3.774	1.00	65.06
	3462	C	LEV B	53	34.357	55.039	5.132	1.00	65.06
	3463	ŏ	LEU B	53	38.775 38.547	55.005 56.209	5.509	1.00	115.15
40	3464	Ň	ASN B	54	39.712	54.549	5.659 4.676	1.00 1.00	115.15
	3465	CA	ASN B	54	40.533	55.488	3.918	1.00	78.33
	3466	CB	ASN B	54	41.826	54.832	3.460	1.00	78.33 116.91
	3467	CG	ASN B	54	42.792	54.609	4.598	1.00	116.91
45	3468	OD1	ASN B	54	43.166	55.545	5.307	1.00	116.91
43	3469	ND2	ASN B	54	43.204	53.364	4.782	1.00	116.91
	3470	C	ASN B	54	39.834	56.084	2.716	1.00	78.33
	3471 3472	O N	ASN B	54	38.853	55.548	2.226	1.00	78.33
	3473	CA	ILE B	5 5	40.333	57.227	2.269	1.00	83.98
50	3474	CB	ILE B	55 55	39.800	57.906 50.444	1.100	1.00	83.98
	3475	CG2	ILE B	55	38.973 38.828	59.141 60.092	1.493	1.00	67.63
	3476	CG1	ILE B	55	37.598	58.686	0.322	1.00	67.63
	3477	CD1	ILE B	55	36.675	59.826	1.980 2.438	1.00	67.63
	3478	С	ILE B	55	41.015	58.329	0.298	1.00 1.00	67.63 83.98
55	3479	0	ILE B	55	41.882	59.043	0.805	1.00	83.98
	3480	N	√AL B	56	41.099	57.866	-0.942	1.00	110.45
	3481	CA	VAL B	56	42.231	58.216	-1.781	1.00	110.45
	3482	CB	VAL B	56	42.737	56.993	-2.541	1.00	102.53
60	3483	CG1	VAL B	56	44.131	57.246	-3.058	1.00	102.53
00	3484 3485	CG2	VAL B	56	42.749	55.791	-1.618	1.00	102.53
	3486	C	VAL B	56	41.796	59.306	-2.748	1.00	110.45
	3487	N	VAL B ASN B	56 57	40.783	59.952	-2.515	1.00	110.45
	3488	CA	ASN B	57 57	42.556 42.235	59.515 60.554	-3.820	1.00	137.41
65	3489	CB	ASN B	57 57	42.235 42.508	60.554	-4.794 C 04.6	1.00	137.41
-	3490	ČĠ	ASN B	57 57	43.990	60.063 59.900	-6.216 -6.403	1.00	211.36
	3491	OD1	ASN B	57	44.776	60.825	-6.493 -6.294	1.00	211.36
	3492	ND2	ASN B	57	44.379	58.721	-6.254 -6.959	1.00 1.00	211.36
	3493	C	ASN B	57	40.795	61.032	-4.667	1.00	211.36 137.41
70	3494	0	ASN B	57	39.885	60.501	-5.305	1.00	137.41
									.57.41

	3495	N	ALA B	58	40,608	62.038	-3.818	1.00	74.20
	3496	CA	ALA B	58	39.303	62.603	-3.561	1.00	74.20 74.20
	3497	CB .	ALA B	58	39.440	63.783	-2.609	1.00	169.14
_	3498	Ç	ALA B	58	38.534	63.034	-4.817	1.00	74.20
5	3499	0	ALA B	58	38.983	63.895	-5.579	1.00	74.20
	3500 3501	N CA	LYS B LYS B	59 50	37.366	62.433	-5.015	1.00	107.95
	3502	CB	LYS B	59 59	36.507 36.037	62.766 61.485	-6.137	1.00	107.95
	3503	ČĞ	LYS B	59	37.184	60.618	-6.837 -7.354	1.00 1.00	214.35
10	3504	CD	LYS B	59	36.703	59.292	-7.930	1.00	214.35 214.35
	3505	CE	LYS B	59	37.872	58.451	-8.432	1.00	214.35
	3506	NZ	LYS B	59	37.428	57.138	-8.972	1.00	214.35
	3507	C	LYS B	59	35.330	63.514	-5.521	1.00	107.95
15	3508 3509	0 N	LYS B PHE B	59	34.924	63.205	-4.397	1.00	107.95
13	3510	CA	PHE B	60 60	34.798 33.670	64.502 65.268	-6.234	1.00	88.51
	3511	CB	PHE B	60	33.032	66.051	-5.716 -6.845	1.00 1.00	88.51
	3512	CG	PHE B	60	33.926	67.085	-7.419	1.00	104.07 104.07
••	3513	CD1	PHE B	60	33.803	67.477	-8.736	1.00	104.07
20	3514	CD2	PHE B	60	34.893	67.682	-6.635	1.00	104.07
	3515	CE1	PHE B	60	34.629	68.451	-9.266	1.00	104.07
	3516 3517	CE2 CZ	PHE B PHE B	60	35.725	68.654	·7.155	1.00	104.07
	3518	C	PHE B	60 60	35.592 32.616	69.038 64.397	-8.473	1.00	104.07
25	3519	ŏ	PHE B	60	31.988	64.816	-5.032 -4.0 6 0	1.00 1.00	88.51
	3520	N	GLU B	61	32.438	63.177	-5.536	1.00	88.51 122.82
	3521	CA	GLU B	61	31.453	62.251	-4.988	1.00	122.82
	3522	CB	GLU B	61	31.362	60.981	- 5. 83 8	1.00	242.03
30	3523	CG	GLU B	61	30.921	61.202	-7.268	1.00	242.03
30	3524 3525	CD OE1	GLU B GLU B	61	31.866	62.107	-8.030	1.00	242.03
	3526	OE2	GLU B	61 61	33.080 31.395	61.812 63.111	-8.056 -8.604	1.00	242.03
	3527	C	GLU B	61	31.772	61.856	-8.5 63	1.00 1.00	242.03 122.82
	3528	Ö	GLU B	61	30.884	61.426	-2.829	1.00	122.82
35	3529	N	ASP B	62	33.038	61.982	-3.173	1.00	75.67
	3530	CA	ASP B	62	33.435	61.622	-1.821	1.00	75.67
	3531 3532	CB	ASP B	62	34.954	61.524	-1.708	1.00	186,17
	3533	CG OD1	ASP B	62 62	35.544 34.918	60.572	-2.723	1.00	186.17
40	3534	OD2	ASP B	62	36.638	59.528 60.860	-2.996 -3.242	1.00 1.00	186.17
	3535	C	ASP B	62	32.889	62.643	-0.834	1.00	186.17 75.67
	3536	0	ASP B	62	32.765	62.359	0.354	1.00	75.67
	3537	N	SER B	63	32.553	63.832	-1.330	1.00	56.90
45	3538	CA	SER B	63	31.993	64.872	-0.471	1.00	56.90
43	3539 3540	CB OG	SER B SER B	63 63	31.659	66.117	-1.286	1.00	0.16
	3541	C	SER B	63 63	32.823 30.710	66.739 64.291	-1.783 0.102	1.00	80.16
	3542	ŏ	SER B	63	29.919	63.744	-0.643	1.00 1.00	56.90 56.90
	3543	N	GLY B	64	30.482	64.385	1.407	1.00	91.31
50	3544	CA	GLY B	64	29.254	63.819	1.941	1.00	91.31
	3545	Ç	GLY B	64	29.177	63.712	3.447	1.00	91.31
	3546 3547	0 N	GLY B	64	30.012	64.259	4.164	1.00	91.31
	3548	CA	GLU B	65 65	28.154	63.014	3.922	1.00	66.19
55	3549	CB	GLU B	65	27.919 26.443	62.813 63.045	5.351 5.642	1.00	66.19
	3550	CG	GLU B	65	25.981	62.639	7.018	1.00 1.00	1°2.59 122.59
	3551	CD	GLU B	65	24.468	62.585	7.107	1.00	122.59
	3552	OE1	GLU B	65	23.856	61.738	6.417	1.00	122.59
60	3553	OE2	GLU B	65	23.890	63.390	7.863	1.00	122.59
UU	3554 3555	C O	GLU B	65 65	28.311	61.374	5.711	1.00	66.19
	3556	Ň	GLU B TYR B	65 66	27.826 29.183	60.434 61.182	5.088 6.607	1.00	66.19
	3557	CA	TYR B	66	29.603	59.833	6.697 7.060	1.00 1.00	58.72 58.72
	3558	CB	TYR B	66	31.093	59.680	6.855	1.00	58.72 55.88
65	3559	CG	TYR B	66	31.576	59.790	5.452	1.00	55.88
	3560	CD1	TYR B	66	31.703	61.020	4.825	1.00	55.88
	3561 3562	CE1	TYR B	66	32.243	61.109	3.548	1.00	55.88
	3563	CD2 CE2	TYR B TYR B	66 66	31.986	58.657	4.772	1.00	55.88
70	3564	CZ	TYR B	66	32.521 32.655	58.726 59.947	3.505 2.896	1.00	55.88 55.88
		- -			w	J3.041	2.030	1.00	55.88

	3565	ОН	TYR B	66	33.230	59.979	1.643	1.00	55.88
	3566	С	TYR B	66	29.320	59.544	8.522	1.00	58.72
	3567	0	TYR B	66	29.111	60.482	9.311	1.00	58.72
_	3568	N	LYS B	67	29.347	58.257	8.884	1.00	128.26
5	3569	CA	LYS B	67	29.129	57.823	10.269	1.00	128.26
	3570	CB	LYS B	67	27.689	58.067	10.679	1.00	129.32
	3571	CG	LYS B	67	26.702	57.535	9.689	1.00	
	3572	CD	LYS B	67	25.301	57.905	10.098	1.00	129.32
	3573	CE	LYS B	67	24.314	57.545	9.007		129.32
10	3574	NZ	LYS B	67	22.936	57.963	9.372	1.00	129.32
••	3575	C	LYS B	67	29.460	56.351		1.00	129.32
	3576	ŏ	LYS B	67			10.466	1.00	128.26
	3577	Ň	CYS B		29.434	55.570	9.516	1.00	128.26
	3578	ČA	CYS B	68	29.793	55.971	11.696	1.00	93.88
15				68	30.107	54.581	11.964	1.00	93.88
13	3579	C	CYS B	68	29.262	54.113	13.122	1.00	93.88
	3580	0	CYS B	68	28.693	54.923	13.850	1.00	93.88
	3581	CB	CYS B	68	31.609	54.381	12.247	1.00	200.62
	3582	SG	CYS B	68	32.359	55.270	13.646	1.00	200.62
20	3583	N	GLN B	69	29.148	52.797	13.255	1.00	198.52
20	3584	CA	GLN B	69	28.375	52.172	14.318	1.00	198.52
	3585	CB	GLN B	69	26.897	52.107	13.926	1.00	207.53
	3586	CG	GLN B	69	26.082	51.114	14.734	1.00	207.53
	3587	CD	GLN B	69	24.654	50.983	14.233	1.00	207.53
	3588	OE1	GLN B	69	24,419	50.759	13.044	1.00	207.53
25	3589	NE2	GLN B	60	23.692	51.117	15.143	1.00	
	3590	С	GLN B	69	28.921	50.768	14.527	1.00	207.53
	3591	0	GLN B	69	29.474	50.173	13.600	1.00	198.52
	3592	Ň	HIS B	70	28.772	50.240			198.52
	3593	CA	HIS B	70	29.266	48.903	15.739	1.00	126.14
30	3594	CB	HIS B	70	30.134		16.020	1.00	126.14
-	3595	CG	HIS B	70		48.915	17.265	1.00	193.31
	3596	CD2			31.435	49.650	. 17.083	1.00	193.31
	3597			70	31.809	50.892	17.450	1.00	193.31
	3598	ND1	HIS B	70	32.502	49.089	16.411	1.00	193.31
35		CE1	HIS B	70	33.480	49.982	16.371	1.00	193.31
33	3599	NE2	HIS B	70	33.095	51.074	16.992	1.00	193.31
	3600	Ç	HIS B	70	28.144	47.890	16.193	1.00	126.14
	3601	0	HIS B	70	26.974	48.180	15.915	1.00	126.14
	3602	N	GLN B	71	28.511	46.697	16.639	1.00	181.78
40	3603	CA	GLN B	71	27.558	45.621	16.836	1.00	181.78
40	3604	CB	GLN B	71	28.277	44.424	17.456	1.00	249.38
	3605	CG	GLN B	71	27.687	43.082	17.057	1.00	249,38
	3606	CD	GLN B	71	27.525	42.946	15.553	1.00	249.38
	3607	OE1	GLN B	71	28.501	42.814	14.816	1.00	249.38
	3608	NE2	GLN B	71	26.283	42,994	15.091	1.00	249.38
45	3609	С	GLN B	71	26.374	46.062	17.711	1.00	181.78
	3610	0	GLN B	71	25.214	45.948	17.300	1.00	181.78
	3611	N	GLN B	72	26.666	46.582	18.902	1.00	249.48
	3612	CA	GLN B	72	25.627	47.029	19.838	1.00	
	3613	CB	GLN B	72	25.631	46.132	21.084	1.00	249.48
50	3614	CG	GLN B	72	24.511	46.421	22.083		225.39
	3615	CD	GLN B	72	24.526	45.478		1.00	225.39
	3616	OE1	GLN B	72	24.436	44.260	23.273	1.00	225.39
	3617	NE2	GLN B	72			23.115	1.00	225.39
	3618	C	GLN B		24.641	46.038	24.471	1.00	225.39
55	3619	ŏ	GLN B	72 70	25.812	48.487	20.262	1.00	249.48
55	3620	Ň	ULIV D	72	25.935	48.787	21.455	1.00	249.48
	3621		VAL B	73	25.821	49.395	19.288	1.00	181.22
	3622	CA	VAL B	73	26.005	50.817	19.583	1.00	181.22
		CB	VAL B	73	27.465	51.205	19.481	1.00	249.28
60	3623	CG1	VAL B	73	27.738	52.552	20.109	1.00	249.28
UU	3624	CG2	VAL B	73	28.193	50.235	20.151	1.00	249.28
	3625	Ç	VAL B	73	25.240	51.690	18.626	1.00	181.22
	3626	0	VAL B	73	25.071	51.348	17.462	1.00	181.22
	3627	N	ASN B	74	24.776	52.826	19.122	1.00	246.14
15	3628	CA ·	ASN B	74	24.042	53.744	18.278	1.00	246.14
65	3629	CB	ASN B	74	23.201	54.681	19.141	1.00	197.13
	3630	CG	ASN B	74	22.296	53.925	20.082	1.00	197.13
	3631	OD1	ASN B	74	21.682	52.931	19.688	1.00	197.13
	3632	ND2	ASN B	74	22.202	54.394	21.324	1.00	197.13
	3633	С	ASN B	74	25.027	54.526	17.418	1.00	
70	3634	0	ASN B	74	26.004	55.081	17.922	1.00	246.14
							*****	1.00	246.14

	3635	N	GLU B	75	24.761	54.542	16.114	1.00	146.48
	3636	CA	GLU B	75	25.597	55.232	15.135	1.00	146.48
	3637	CB	GLU B	75	24.848	55.331	13.807	1.00	234.88
5	3638	CG	GLU B	75	23.346	55.500	13.966	1.00	234.88
)	3639	CD	GLU B	75	22.604	55.365	12.648	1.00	234.88
	3640	OE1	GLU B	75	22.784	54.328	11.970	1.00	234.88
	3641 3642	OE2	GLU B	75 75	21.840	56.291	12.295	1.00	234.88
	3643	C	GLU B GLU B	75 76	26.075	56.613	15.579	1.00	146.48
10	3644	N	SER B	75 76	25.344	57.361	16.239	1.00	146,48
	3645	ĞA	SER B	76 76	27.311 27.958	56.939 58.200	15.201	1.00	102.01
	3646	CB	SER B	76	29.420	58.153	15.564 15.147	1.00	102.01
	3647	ÖĞ	SER B	76	29.501	58.098	13.732	1.00 1.00	220.64
	3648	Č	SER B	76	27.336	59.426	14.930	1.00	220.64
15	3649	0	SER B	76	26.652	59.332	13.921	1.00	102.01 102.01
	3650	N	GLU B	77	27.604	60.583	15.522	1.00	133.62
	3651	CA	GLU B	77	27.102	61.838	14.988	1.00	133.62
	3652	CB	GLU B	77	27.429	62.993	15.941	1.00	240.61
20	3653	CG	GLU B	77	26.732	62.894	17.288	1.00	240.61
20	3654	CD	GLU B	77	25.218	62. 99 5	17.179	1.00	240.61
	3655	OE1	GLU B	77	24.686	62.847	16.060	1.00	240.61
	3656	OE2	GLU B	77	24.558	63.213	18.217	1.00	240.61
	3657 3658	C	GLU B	<u> 77</u>	27.798	62.057	13.651	1.00	133.62
25	3659	. N	GLU B	77	29.023	62.177	13.597	1.00	133.62
25	3660	CD	PRO B PRO B	78 70	27.030	62.096	12.549	1.00	89.52
	3661	CA	PRO B	78 78	25.577 27.543	61.836 62.294	12.507	1.00	87.18
	3662	CB	PRO B	78	26.295	62.633	11.196	1.00	89.52
	3663	ČĞ	PRO B	78	25.313	61.698	10.408 11.009	1.00	87.18
30	3664	Č	PRO B	78	28.586	63.370	11.009	1.00 1.00	87.18
	3665	Ö	PRO B	78	28.644	64.258	11.943	1.00	89.52
	3666	N	VAL B	79	29.430	63.270	10.082	1.00	89.52 99.13
	3667	CA	VAL B	79	30.475	64.256	9.872	1.00	99.13
	3668	CB	VAL B	79	31.833	63.720	10,291	1.00	115.84
35	3669	CG1	VAL B	79	32.929	64.618	9.749	1.00	115.84
	3670	CG2	VAL B	79	31.908	63.671	11.798	1.00	115.84
	3671	C	VAL B	79	30.512	64.571	8.401	1.00	99.13
	3672	0	VAL B	79	30.573	63.654	7.592	1.00	99.13
40	3673 3674	N CA	TYR B	80	30.480	65.853	8.044	1.00	70.58
40	3675	CB	TYR B TYR B	80	30.490	66.213	6.637	1.00	70.58
	3676	CG	TYR B	80 80	29.622 29.319	67.426 67.534	6.352	1.00	173.93
	3677	CD1	TYR B	80	28.546	67.524 66.550	4.884 4.261	1.00	173.93
	3678	CE1	TYR B	80	28.266	66.604	2.913	1.00 1.00	173.93
45	3679	CD2	TYR B	80	29.824	68.559	4.106	1.00	173.93 173.93
	3680	CE2	TYR B	80	29.561	68.613	2.729	1.00	173.93
	3681	CZ	TYR B	80	28.769	67.630	2.148	1.00	173.93
	3682	OH	TYR B	80	28.432	67.702	0.811	1.00	173.93
50	3683	С	TYR B	:0	31.858	66.511	6.103	1.00	70.58
50	3684	0	TYR B	80	32.657	67.183	6.739	1.00	70.58
	3685	N	LEU B	81	32.109	66.033	4.902	1.00	86.81
	3686	CA	LEU B	81	33.375	66.256	4.254	1.00	86.81
	3687	CB	LEU B	81	34.030	64.899	3.970	1.00	52.23
55	3688 3689	CG CD1	LEU B	81	35.301	65.038	3.148	1.00	52.23
55	3690	CD1 CD2	LEU B	81	36.303	65.810	3.970	1.00	52.23
	3691	C	LEU B	81 81	35.843 33.090	63.724	2.783	1.00	52.23
	3692	ŏ	LEU B	81	32.240	66.999 66.576	2.944	1.00	86.81
	3693	Ň	GLU B	82	33.777	68.104	2.171 2.682	1.00	86.81
60	3694	CA	GLU B	82	33.537	68.808	1.430	1.00 1.00	81.52 81.52
	3695	CB	GLU B	82	33.000	70.212	1.700	1.00	166.15
	3696	CG	GLU B	82	32.168	70.757	0.552	1.00	166.15
	3697	CD	GLU B	82	31.619	72.139	0.827	1.00	166.15
15	3698	OE1	GLU B	82	31.239	72.409	1.988	1.00	166.15
65	3699	OE2	GLU B	82	31.557	72.953	-0.118	1.00	166.15
	3700	Ç	GLU B	82	34.800	68.898	0.584	1.00	81.52
	3701	0	GLU B	82	35.856	69.283	1.072	1.00	81.52
	3702	N	VAL B	83	34.691	68.555	-0.692	1.00	81.14
70	3703	CA	VAL B	83	35.842	68.595	-1.584	1.00	81.14
10	3704	СВ	VAL B	83	35.910	67.346	-2.417	1.00	54.13

	3705	CG1	VAL B	83-	37.014	67.472	.2.422	4.00	
	3706	CG2	VAL B	83	36.159	66.136	-3.433 -1.512	1.00	54.13
	3707	c	VAL B	83	35.848	69.781	-1.512 -2.535	1.00	54.13
	3708	ō.	VAL B	83	34.831	70.075	-3.168	1.00 1.00	81.14
5	3709	N	PHE B	84	37.000	70.441	-2.667	1.00	81.14
	3710	CA	PHE B	84	37 NR4	71.612	-3.530	1.00	61.79
	3711	CB	PHE B	84	37.407	72.864	-2.729	1.00	61.79
	3712	CG	PHE B	84	36.432	73.162	-1.660	1.00	77.82 77.82
	3713	CD1	PHE B	84	36.408	72.410	-0.500	1.00	77.82 77.82
10	3714	CD2	PHE B	84	35.555	74.223	-1.790	1.00	77.82
	3715	CE1	PHE B	84	35.513	72.699	0.522	1.00	77.82
	3716	CE2	PHE B	84	34.650	74.529	-0.779	1.00	77.82
	3717	CZ	PHE B	84	34.634	73.766	0.384	1.00	77.82
15	3718	C	PHE B	84	38.081	71.568	-4.654	1.00	61.79
15	3719	0	PHE B	84	38.978	70.728	-4.701	1.00	61.79
	3720	N	SER B	85	37.893	72.538	-5.543	1.00	129.28
	3721	CA	SER B	85	38.736	72.777	-6.696	1.00	129.28
	3722	CB	SER B	85	38.066	72.284	-7.980	1.00	132.41
20	3723	og	SER B	85	38.879	72.526	-9.116	1.00	132.41
20	3724	C	SER B	85	38.840	74.296	-6.713	1.00	129.28
	3725	0	SER B	85	37.845	74.988	-6.967	1.00	129.28
	3726	N	ASP B	86	40.026	74.811	-6.395	1.00	77.53
	3727	CA	ASP B	86	40.255	76.257	-6.385	1.00	77.53
25	3728 3729	CB CG	ASP B	86	39.348	76.933	-5.354	1.00	206.86
25	3729 3730		ASP B	86	38.874	78.300	-5.809	1.00	206.86
	3731	OD1 OD2	ASP B	86	39.733	79.139	-6.163	1.00	206.86
	3732	C	ASP B ASP B	86	37.644	78.535	-5.812	1.00	206.86
	3733	ŏ	ASP B	86	41.719	76.537	-6.065	1.00	77.53
30	3734	N	TRP B	86	42.423	75.643	-5.601	1.00	77.53
50	3735	CA	TRP B	87 87	42.186 43.589	77.759	-6.313	1.00	63.09
	3736	CB	TRP B	87	43.934	78.072	-6.048	1.00	63.09
	3737	CG	TRP B	87	44.332	79.488 79.502	-6.505 -7.919	1.00	213.86
	3738	CD2	TRP B	87	43.467	79.711	-7.919 -9.031	1.00	213.86
35	3739	CE2	TRP B	87	44.225	79.492	-10.196	1.00 1.00	213.86
	3740	CE3	TRP B	87	42.115	80.053	-9.157	1.00	213.86
	3741	CD1	TRP B	87	45.561	79.186	-8.435	1.00	213.86
	3742	NE1	TRP B	87	45.500	79.175	-9.807	1.00	213.86 213.86
	3743	CZ2	TRP B	87	43.674	79.604	-11.468	1.00	213.86
40	3744	CZ3	TRP B	87	41.570	80.162	-10.423	1.00	213.86
	3745	CH2	TRP B	87	42.347	79.943	-11.559	1.00	213.86
	3746	C	TRP B	87	43.913	77.935	-4.589	1.00	63.09
	3747	0	TRP B	87	44.856	77.221	-4.208	1.00	63.09
4.5	3748	N	LEU B	88	43.110	78.622	-3.783	1.00	95.94
45	3749	CA	LEU B	88	43.280	78.617	-2.349	1.00	95.94
	3750	CB	LEV B	88	43.600	80.021	-1.861	1.00	93.07
	3751	CG	LEU B	88	44.931	80.558	-2.32 5	1.00	93.07
	3752	CD1	LEU B	88	45.167	81.882	-1.668	1.00	93.07
50	3753	CD2	LEU B	88	46.019	79.559	-1.955	1.00	93.07
20	3754	C	LEU B	88	42.050	78.126	-1.621	1.00	95.94
	3755	0	LEU B	88	40.927	78.425	-2.004	1.00	95.94
	3756	N	LEU B	89	42.276	77.380	-0.550	1.00	57.56
	3757	CA	LEU B	89	41.191	76.863	0.265	1.00	57.56
55	3758	CB	LEU B	89	41.063	75.370	0.059	1.00	98.29
55	3759 3760	CG	LEU B	89	39.972	74.802	0.940	1.00	98.29
	3761	CD1	LEU B	89	38.700	75.640	0.767	1.00	98.29
	3762	CD2	LEV B	89	39.741	73.357	0.564	1.00	98.29
	3763	C	LEU B LEU B	89	41.488	77.138	1.724	1.00	57.56
60	3764	N	LEU B	89	42.566	76.832	2.192	1.00	57.56
•	3765	CA	LEU B	90	40.553	77.737	2.444	1.00	82.03
	3766	CB	LEU B	90	40.787	78.008	3.857	1.00	82.03
	37 6 7	CG	LEU B	90	40.005	79.244	4.303	1.00	51.54
	3768	CD1	LEU B	90 90	40.073	79.537	5.807	1.00	51.54
65	3769	CD2	LEU B	90 90	41.486	79.805	6.154	1.00	51.54
	3770	C	LEU B	90	39.203 40.347	80.720 76.808	6.203	1.00	51.54
	3771	ŏ	LEU B	90			4.674	1.00	82.03
	3772	Ň	GLN B	91	39.173 41.274	76.431 76.199	4.667 5.301	1.00	82.03
	3773	CA	GLN B	91	40.904	75.024	5.391 6.182	1.00	55.00
70	3774	CB	GLN B	91	41.909	73.900	5.955	1.00	55.00 70.63
		_		- •		. 0.000	5.855	1.00	79.62

	3775	CG	GLN B	91-	42.017	73.500	4.501	1.00	79.62
	3776	CD	GLN B	91	42.871	72.287	4.316	1.00	79.62
	3777	OE1	GLN B	91	44.072	72.334	4.524	1.00	79.62
5	3778 3779	NE2	GLN B GLN B	91	42.253	71.180	3.942	1.00	79.62
,	3779	CO	GLN B	91 91	40.793 41.552	75.316 76.118	7.670	1.00	55.00
	3781	Ň	ALA B	92	39.846	74,680	8.212 8.344	1.00 1.00	55.00
	3782	ĈA	ALA B	92	39.692	74.939	9.760	1.00	72.63
	3783	CB	ALA B	92	38.406	75.678	10.004	1.00	72.63 131.49
10	3784	С	ALA B	92	39.691	73.632	10.519	1.00	72.63
	3785	0	ALA B	92	39.122	72,634	10.050	1.00	72.63
	3786	N	SER B	93	40.338	73.624	11.685	1.00	73.84
	3787	CA	SER B	93	40.381	72,421	12.512	1.00	73.84
15	3788 3789	CB OG	SER B	93	41.018	72.709	13.873	1.00	152.84
13	3790	C	SER B SER B	93 93	40.445 38.934	73.845 72.013	14.491	1.00	152.84
	3791	ŏ	SER B	93	38.515	70.973	12.691 12.179	1.00 1.00	73.84
	3792	Ň	ALA B	94	38.167	72.859	13.378	1.00	73.84 105.05
	3793	CA	ALA B	94	36.743	72.624	13.619	1.00	105.05
20	3794	CB	ALA B	94	36.517	72.246	15.061	1.00	185.57
	3795	Ç	ALA B	94	35.978	73.898	13.280	1.00	105.05
	3796	0	ALA B	94	36.478	74.988	13.524	1.00	105.05
	3797 3798	N CA	GLU B GLU B	95 05	34.776	73.763	12.724	1.00	101.72
25	3799	CB	GLU B	95 95	34.005 33.081	74.936	12.340	1.00	101.72
23	3800	CG	GLU B	95	33.822	74.601 74.120	11.175 9.941	1,00 1.00	160.65
	3801	CD	GLU B	95	32.955	74.120	8.692	1.00	160.65 160.65
	3802	OE1	GLU B	95	33.455	73.705	7.625	1.00	160.65
	3803	OE2	GLU B	95	31.779	74.538	8.771	1.00	160.65
30	3804	C	GLU B	95	33.205	75.550	13.473	1.00	101.72
	3805	0	GLU B	95	32.732	76.677	13.354	1.00	101.72
	3806 3807	N CA	VAL B VAL B	96 06	33.050	74.807	14.565	1.00	87.11
	3808	CB	VAL B	96 96	32.322 30.947	75.296 74.746	15.730 15.781	1.00	87.11
35	3809	CG1	VAL B	96	30.147	74.746 75.595	16.714	1.00 1.00	166.75 166.75
	3810	CG2	VAL B	96	30.349	74.728	14.367	1.00	166.75
	3811	C	VAL B	96	33.096	74.866	16.955	1.00	87.11
	3812	0	VAL B	96	33.528	73.724	17.052	1.00	87.11
40	3813	N	VAL B	97	33.260	75.781	17.900	1.00	103.60
40	3814	CA CB	VAL B	97	34.080	75.505	19.067	1.00	103.60
	3815 3816	CG1	VAL B VAL B	97 97	35.444 36.415	76.140 75.600	18.858	1.00	67.08
	3817	CG2	VAL B	97	35.924	75.622 75.882	19.857 17.456	1.00 1.00	67.08 67.09
	3818	c	VAL B	97	33.591	76.003	20.417	1.00	67.08 103.60
45	3819	0	VAL B	97	33.142	77.136	20.533	1.00	103.60
	3820	N	MET B	98	33.730	75.168	21.441	1.00	173.13
	3821	CA	MET B	98	33.341	75.542	22.798	1.00	173.13
	3822	CB	MET B	98	33.361	74.306	23.696	1.00	240.86
50	3823 3824	CG SD	MET B	98	32.369	73.237	23.290	1.00	240.86
50	3825	CE	MET B	98 98	30. 722 30.921	73.639 73.267	23.866 25.612	1.00 1.00	240.86
	3826	Č	MET B	98	34.341	76.573	23.323	1.00	240.86 1 73 .13
	3827	0	MET B	98	35.547	76.380	23.185	1.00	173.13
	3828	N	GLU B	99	33.849	77.658	23.918	1.00	116.59
55	3829	CA	GLU B	99	34.731	78.695	24.451	1.00	116.59
	3830	CB	GLU B	99	33.954	79.631	25.376	1.00	249.41
	3831	CG	GLU B	99	34.610	80.985	25.567	1.00	249.41
	3832 3833	CD OE1	GLU B	99	34,016	81.763	26.727	1.00	249.41
60	3834	OE2	GLU B	99 99	32.782 34.781	81.690 82.455	26.920 27.435	1.00	249.41
-	3835	Č	GLU B	99	35.853	78.023	25.247	1.00 1.00	249.41 116.59
	3836	ŏ	GLU B	99	35.582	77.203	26.127	1.00	116.59
	3837	N	GLY B	100	37.106	78.351	24.935	1.00	84.75
CF	3838	CA	GLY B	100	38.221	77.751	25.651	1.00	84.75
65	3839	C	GLY B	100	39.031	76.722	24.883	1.00	84.75
	3840	O .	GLY B	100	40.171	76.451	25.243	1.00	84.75
	3841 3842	N CA	GLN B GLN B	101	38.464	76.151 76.134	23.824	1.00	108.09
	3843	CB	GLN B	101 101	39.167 38.151	75.134 74.231	23.033 22.324	1.00	108.09
70	384-1	ČĞ	GLN B	101	37.313	73.397	23.267	1.00 1.00	249.17 249.17
									~70.17

	3845 3846 3847 3848 5 3849 3850 3851	OI NE	E1 GLN E2 GLN GLN GLN PRO	B B B	101 101 101 101 102	38.163 38.643 38.370 40.159 40.186 40.996	72.685 73.292 71.395 75.687 76.880 74.815	25 24 22 21.	.297 1.0 .255 1.0 .094 1.0 .000 1.0 .723 1.0	249.17 249.17 20 249.17 20 108.09
	3852 3853 3854 3855 3856	CA CB CG C	PRO PRO	8 8 8	102 4 102 4	41.175 41.948 43.006 42.177 41.270	73.371 75.301 74.212 72.979 75.466	21. 20. 20. 20.	431 1.00 592 1.00	0 84.30 0 171.21 0 84.30 0 171.21
	3857 3858 3859 3860 3861	N CA CB CG CD1	LEU LEU LEU	B B B	103 4 103 4 103 4	0.260 1.828 1.299 0.437 9.866	74.799 76.351 76.588 77.830 78.063	19.0 18.7 18.2 16.9 16.9	745 1.00 128 1.00 100 1.00 10 1.00	84.30 84.30 75.78 75.78
2	3862 3863 20 3864 3865 3866	CD2 C O N	LEU LEU (PHE (8 B B	103 38 103 39 103 42 103 43	3.942 9.117 9.411 9.216 9.470	76.897 79.391 76.793 77.686	15.5 15.14 15.48 15.89	15 1.00 42 1.00 33 1.00 92 1.00	79.40 79.40 79.40 79.40 75.78
2	3867 3868 3869 3870 3871	CA CB CG CD1 CD2	PHE E PHE E PHE E PHE B	3 1 3 1 1 1	104 43 104 44 104 45 04 44	.524 .441 .088 366 423	75.993 76.182 74.953 74.577 73.908	14.82 13.83 13.75 15.05 16.03	1.00 18 1.00 2 1.00 4 1.00	75.78 73.92 73.92 179.34 179.34
30	3872 3873	CE1 CE2 CZ C	PHE B PHE B PHE B PHE B PHE B	1 1: 1:	04 44. 04 47. 04 46. 04 42.	960 028 295 958	74.880 73.550 74.527 73.857 76.472	15.299 17.248 16.512 17.485 12.448	9 1.00 3 1.00 2 1.00 5 1.00	179.34 179.34 179.34 179.34 179.34
35	3877 3878	N CA CB CG CD1	LEU B LEU B LEU B LEU B	10 10 10 10	05 43.3 05 42.9 05 42.5 05 41.4	187 185 103 09	75.717 77.581 77.920 79.354 79.667	11.947 11.838 10.468 10.385 11.381	1.00	73.92 73.92 49.92 49.92 78.62
40	3882 3883 3884 3885	CD2 C O N CA	LEU B LEU B LEU B ARG B ARG B	10: 10: 10: 10: 10:	5 40.3 5 44.2 5 45.3 6 44.0	68 24 27 51	81.064 78.612 77.773 78.095 77.317	11.137 11.223 9.580 9.991 8.355	1.00 1.00 1.00 1.00	78.62 78.62 78.62 49.92 49.92
45	3886 3887 3888 3889 3890	CB CG CD NE CZ	ARG B ARG B ARG B ARG B ARG B	106 106 106	45.53 46.63 46.73 47.76	17 13 18 7	77.131 75.649 75.284 73.775 73.414	7.494 7.475 6.526 6.383	1.00 1.00 1.00 1.00 1.00	79.70 79.70 126.47 126.47 126.47
50	3891 3892 3893 3894 3895	NH1 NH2 C O N	ARG B ARG B ARG B ARG B	106 106 106 106 106	46.86	2 7 9 7 8 7	2.255 1.343 2.018 7.615 7.192	5.412 4.773 5.006 3.891 6.083	1.00 1.00 1.00 1.00 1.00	126.47 126.47 126.47 126.47 126.47 79.70
55	3896 3897 3898 3899 3900 3901	CA C O CB SG	CYS B CYS B CYS B CYS B CYS B CYS B	107 107 107 107 107 107	45.730 45.507 46.217 47.442 46.087 45.402	70 77 77 77 80	8.518 3.971 7.938 7.869 0.353	5.483 5.553 4.177 3.331 3.318 3.919	1.00 1.00 1.00 1.00 1.00 1.00	79.70 64.58 64.58 64.58 64.58
60	3902 3903 3904 3905 3906	N CA CB OG CD2	HIS B HIS B HIS B HIS B	108 108 108 108 108	45.435 45.970 45.151 45.702 45.138	77 76 74, 73.	.142 .124 .037 .790 548	2.422 2.639 1.845 2.131 1.513	1.00 1.00 1.00 1.00 1.00	107.35 107.35 77.57 77.57 100.22
65	3907 3908 3909 3910 3911	ND1 CE1 NE2 C	HIS B HIS B HIS B HIS B	108 108 108 108 108	46.977 47.170 46.070 46.002	73. 71.: 71.: 76.:	645 296	0.691 1.776 1.149 0.483 0.352	1.00 1.00 1.00 1.00	100.22 100.22 100.22 100.22 100.22
70	3912 3913 3914	N CA C	GLY B	109 109 109 109	44.981 47.180 47.338 47.018 47.115	76.6 76.0 76.3 75.0 73.9	079 103 157.	-0.262 -0.231 -1.652 -2.430 -1.886	1.00 1.00 1.00 1.00 1.00	77.57 77.57 82.92 82.92 82.92 82.92

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3973 CG1 VAL B 115 49.833 81.905 -0.946 1.00 112.10 3974 CG2 VAL B 115 49.830 79.436 -1.155 1.00 112.10 3975 C VAL B 115 52.767 81.723 -0.451 1.00 97.38 3976 O VAL B 115 53.333 81.428 0.613 1.00 97.38 3977 N TYR B 116 52.804 82.940 -0.985 1.00 76.30 3978 CA TYR B 116 53.547 84.019 -0.335 1.00 76.30 3979 CB TYR B 116 54.745 84.433 -1.206 1.00 116.08 3980 CG TYR B 116 55.750 82.529 -2.581 1.00 116.08 3981 CD1 TYR B 116 56.63										
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3976 O VAL B 115 53.333 81.428 0.613 1.00 97.38 3977 N TYR B 116 52.804 82.940 -0.985 1.00 76.30 3978 CA TYR B 116 53.547 84.019 -0.335 1.00 76.30 5 3979 CB TYR B 116 54.745 84.433 -1.206 1.00 116.08 3980 CG TYR B 116 55.758 83.328 -1.431 1.00 116.08 3981 CD1 TYR B 116 55.720 82.529 -2.581 1.00 116.08 3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08	60			VAL B	115	49.830	79.436			
3977 N TYR B 116 52.804 82.940 -0.985 1.00 76.30 3978 CA TYR B 116 53.547 84.019 -0.335 1.00 76.30 65 3979 CB TYR B 116 54.745 84.433 -1.206 1.00 116.08 3980 CG TYR B 116 55.758 83.328 -1.431 1.00 116.08 3981 CD1 TYR B 116 55.720 82.529 -2.581 1.00 116.08 3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08								-0.451	1.00	97.38
3978 CA TYR B 116 53.547 84.019 -0.335 1.00 76.30 55 3979 CB TYR B 116 54.745 84.433 -1.206 1.00 116.08 3980 CG TYR B 116 55.758 83.328 -1.431 1.00 116.08 3981 CD1 TYR B 116 55.720 82.529 -2.581 1.00 116.08 3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08										
65 3979 CB TYR B 116 54.745 84.433 -1.206 1.00 116.08 3980 CG TYR B 116 55.758 83.328 -1.431 1.00 116.08 3981 CD1 TYR B 116 55.720 82.529 -2.581 1.00 116.08 3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08				TYPR						
3980 CG TYR B 116 55.758 83.328 -1.431 1.00 116.08 3981 CD1 TYR B 116 55.720 82.529 -2.581 1.00 116.08 3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08	65									
3981 CD1 TYR B 116 55.720 82.529 -2.581 1.00 116.08 3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08		3980	CG	TYR B						
3982 CE1 TYR B 116 56.634 81.486 -2.770 1.00 116.08 3983 CD2 TYR B 116 56.736 83.061 -0.476 1.00 116.08					116	55.720	82.529			
7() 0004 000									1.00	
10 57.057 82.024 -0.650 1.00 116.08	70									
	. •	JJ04	- Care	11N D	110	37.03/	02.U24	-0.650	1.00	116.08

	3985	cz	TYR B	118	57.602	81.238	-1.798	4.00	
	3986	OH	TYR B	116	58.498	80.201	-1.798 -1.964	1.00	116.08
	3987	Ċ.	TYR B	116	52.654	85.227	-0.059	1.00 1.00	116.08
_	3988	o ·	TYR B	116	51.502	85.276	-0.514	1.00	76.30
5	3989	N	LYS B	117	53.193	86.190	0.692	1.00	76.30 87.81
	3990	CA	LYS B	117	52.463	87.411	1.036	1.00	87.81
	3991	СВ	LYS B	117	52.371	88.354	-0.171	1.00	224.81
	3992	CG	LYS B	117	53.560	89.283	-0.373	1.00	224.81
10	3993	CD	LYS B	117	53.183	90.436	-1.295	1.00	224.81
10	3994	CE	LYS B	117	52.028	91.248	-0.711	1.00	224.81
	3995	NZ	LYS B	117	51.604	92.373	-1.593	1.00	224.81
	3996 3997	· C	LYS B	117	51.059	87.049	1.489	1.00	87.81
	3998	N	LYS B VAL B	117	50.060	87.542 86.104	0.946	1.00	87.81
15	3999	CA	VAL B	118 118	50.983 49.696	86.194 85.737	2.498	1.00	60.09
	4000	CB .	VAL B	118	49.815	84.344	2.994 3.577	1.00	60.09
	4001	CG1	VAL B	118	48.782	84.141	4.647	1.00	85.68
	4002	CG2	VAL B	118	49.604	83.325	2.485	1.00 1.00	85.68 85.68
	4003	С	VAL B	118	49.066	86.622	4.034	1.00	60.09
20	4004	0	VAL B	118	49.752	87.066	4.963	1.00	60.09
	4005	N	ILE B	119	47.753	86.837	3.901	1.00	64.26
	4006	CA	ILE B	119	47.003	87.686	4.830	1.00	64.26
	4007	CB	ILE B	119	46.704	89.027	4.196	1.00	68.56
25	4008	CG2	ILE B	119	46.039	89.920	5.184	1.00	68.56
25	4009	CG1	ILE B	119	47.998	89.654	3.705	1.00	68.56
	4010	CD1	ILE B	119	47.766	90.828	2.843	1.00	68.56
	4011 4012	C O	ILE B	119	45.672	87.052	5.173	1.00	64.26
	4013	N	ILE B	119	44.890	86.771	4.259	1.00	64.26
30	4014	ČA	TYR B	120 120	45.402 44.110	86.803	6.458	1.00	74.17
50	4015	CB	TYR B	120	44.176	86.216 85.345	6.816 8.066	1.00	74.17
	4016	CG	TYR B	120	44.901	84.067	7.887	1.00 1.00	67.28
	4017	CD1	TYR B	120	46.269	84.024	8.002	1.00	67.28 67.28
	4018	CE1	TYR B	120	46.975	82.840	7.818	1.00	67.28
35	4019	CD2	TYR B	120	44.225	82.896	7.582	1.00	67.28
	4020	CE2	TYR B	120	44.909	81.695	7.390	1.00	67.28
	4021	CZ	TYR B	120	46.286	81.680	7.511	1.00	67.28
	4022	ОH	TYR B	120	46. 96 6	80.507	7.340	1.00	67.28
40	4023	C	TYR B	120	43.185	87.348	7.125	1.00	74.17
40	4024	0	TYR B	120	43.613	88.351	7.669	1.00	74.17
	4025 4026	N CA	TYR B	121	41.916	87.180	6.799	1.00	60.66
	4027	CB	TYR B	121 121	40.938	88.213	7.080	1.00	60.66
	4028	CG	TYR B	121	40.355 41.299	88.760 89.557	5.776	1.00	108.81
45	4029	CD1	TYR B	121	42.398	88.961	4.908 4.308	1.00 1.00	108.81
_	4030	CE1	TYR B	121	43.239	89.678	3.449	1.00	108.81 108.81
	4031	CD2	TYR B	121	41.058	90.900	4.640	1.00	108.81
	4032	CE2	TYR B	121	41.890	91.629	3.788	1.00	108.81
	4033	CZ	TYR B	121	42.976	91.009	3.195	1.00	108.81
50	4034	ОН	TYR B	121	43.794	91.710	2.340	1.00	108.81
	4035	Č	TYR B	121	39.781	87.692	7.936	1.00	60.66
	4036	0	TYR B	121	39.301	86.560	7.736	1.00	60.66
	4037	N	LYS B	122	39.332	88.510	8.885	1.00	76.13
55	4038 4039	CA	LYS B	122	38.15.⊹	88.138	9.715	1.00	76.13
55	4040	CB CG	LYS B	122	38.594	87.874	11.168	1.00	102.31
	4041	CD	LYS B	122 122	37.410 37. 73 8	87.462 87.500	12.032	1.00	102.31
	4042	ČE	LYS B	122	36.509	87.523 87.285	13.489 14.327	1.00	102.31
	4043	NZ	LYS B	122	36.834	87.504	15.762	1.00 1.00	102.31
60	4044	C	LYS B	122	37.200	89.289	9.679	1.00	102.31 76.13
	4045	0	LYS B	122	37.507	90.390	10.145	1.00	76.13
	4046	N	ASP B	123	36.013	89.034	9.131	1.00	98.55
	4047	CA	ASP B	123	34.968	90.049	9.023	1.00	98.55
<i>C</i>	4048	CB	ASP B	123	34.492	90.473	10.414	1.00	136.85
65	4049	CG	ASP B	123	33.604	89.429	11.059	1.00	136.85
	4050	OD1	ASP B	123	32.692	88.925	10.363	1.00	136.85
	4051	OD2	ASP B	123	33.810	89.122	12.256	1.00	136.85
	4052	C	ASP B	123	35.420	91.268	8.217	1.00	98.55
70	4053 4054	0 N	ASP B	123	35.168	92.418	8.597	1.00	98.55
, ,		••	GLY B	124	36.094	90.997	7.099	1.00	109.74

	4055 4056	CA C	GLY B	124 124	36.578 37.817	92.050 92.800	6.224	1.00	109.74
	4057	ŏ	GLY B	124	38.371	93.600	6.688 5.938	1.00 1.00	109.74
_	4058	N ·	GLU B	125	38.269	92.542	7.911	1.00	109.74 80.11
5	4059	CA	GLU B	125	39.438	93.230	8.468	1.00	80.11
	4060	CB	GLU B	125	39.276	93.432	9.990	1.00	173.35
	4061 4062	CG CD	GLU B	125 125	38.192 38.621	94.412 95.865	10.446	1.00	173.35
	4063	OE1	GLU B	125	39.591	96.256	10.344 11.030	1.00 1.00	173.35
10	4064	OE2	GLU B	125	37.982	96.615	9.577	1.00	173.35 173.35
	4065	Ç	GLU B	125	40.723	92.462	8.243	1.00	80.11
	4066 4067	0 N	GLU B	125	40.728	91.235	8.308	1.00	80.11
	4068	CA	ALA B ALA B	126 126	41.817 43.101	93.171 92.501	7.986 7.826	1.00	116.19
15	4069	СВ	ALA B	126	44.165	93.513	7.450	1.00 1.00	116.19 157.65
	4070	С	ALA B	126	43.385	91.901	9.216	1.00	116.19
	4071	0	ALA B	126	43.051	92.516	10.227	1.00	116.19
	4072 4073	N CA	LEU B	127 127	43.985 44.246	90.715	9.286	1.00	101.69
20	4074	CB	LEU B	127	43.383	90.109 88.875	10.586 10.761	1.00 1.00	101.69
	4075	CG	LEU B	127	43.207	88.660	12.259	1.00	85.89 85.89
	4076	CD1	LEU B	127	42.594	89.929	12.853	1.00	85.89
	4077	CD2	LEU B	127	42.337	87.450	12.551	1.00	85.89
25	4078 4079	C O	LEU B	127 127	45.696 46.240	89.750 90.197	10.902	1.00	101.69
 5	4080	Ň	LYS B	128	46.306	88.916	11.910 10.070	1.00 1.00	101.69 84.42
	4081	CA	LYS B	128	47.701	88.530	10.256	1.00	84.42
	4082	СВ	LYS B	128	47.794	87.118	10.847	1.00	200.20
30	4083 4084	CG	LYS B	128	47.160	86.955	12.220	1.00	200,20
50	4085	CD CE	LYS B	128 128	47.968 47.352	87.634 87.350	13.317 14.684	1.00	200.20
	4086	NZ	LYS B	128	48.172	87.864	15.817	1.00 1.00	200.20 200.20
	4087	С	LYS B	128	48.360	88.558	8.877	1.00	84.42
35	4088	0	LYS B	128	47.675	88.404	7.853	1.00	84.42
23	4089 4090	N CA	TYR B	129 129	49.675 50.387	88.750	8.839	1.00	107.40
	4091	CB	TYR B	129	50.519	88.773 90.208	7.566 7.067	1.00 1.00	107.40 112.63
	4092	CG	TYR B	129	51.618	90.368	6.043	1.00	112.63
40	4093	CD1	TYR B	129	51.417	90.021	4.712	1.00	112.63
40	4094 4095	CE1 CD2	TYR B	129	52.442	90.116	3.781	1.00	112.63
	4096	CE2	TYR B TYR B	129 129	52.879 53.915	90.814 90.911	6.422 5.502	1.00 1.00	112.63
	4097	CZ	TYR B	129	53.693	90.562	4.183	1.00	112.63 112.63
45	4098	ŌН	TYR B	129	54.719	90.665	3.260	1.00	112.63
45	4099	C	TYR B	129	51.779	88.146	7.621	1.00	107.40
	4100 4101	O N	TYR B	129 130	52.518 52.138	88.373 87.376	8.575	1.00	107.40
	4102	CA	TRP B	130	53.454	86.735	6.587 6.524	1.00 1.00	87.42 87.42
~~	4103	СВ	TRP B	130	53.400	85.311	7.090	1.00	190.57
50	4104	CG	TRP B	130	52.744	85.171	8.423	1.00	190.57
	4105 4106	CD2 CE2	TRP B	130	53.401	84.954	9.674	1.00	190.57
	4107	CE3	TRP B	130 130	52.392 54.746	84.829 84.861	10.658 10.062	1.00 1.00	190.57
	4108	CD1	TRP B	130	51.406	85.166	8.687	1.00	190.57 190.57
55	4109	NE1	TRP B	130	51.185	84.959	10.025	1.00	190.57
	4110	CZ2	TRY B	130	52.686	84.607	12.010	1.00	190.57
	4111 4112	CZ3 CH2	TRP B	130 130	55.041 54.011	84.641 84.510	11.412	1.00	190.57
	4113	C	TRP B	130	53.968	86.652	12.366 5.085	1.00 1.00	190.57 87.42
60	4114	0	TRP B	130	53.209	86.847	4.127	1.00	87.42
	4115	N	TYR B	131	55.259	86.362	4.940	1.00	97.57
	4116	CA CB	TYR B	131	55.848	86.212	3.621	1.00	97.57
	4117 4118	CB CG	TYR B TYR B	131 131	57.339 57.881	86.504 86.590	3.647 2.250	1.00	249.42
65	4119	CD1	TYR B	131	57.611	87.707	1.453	1.00 1.00	249.42 249.42
	4120	CE1	TYR B	131	57.982	87.746	0.133	1.00	249.42
	4121	CD2	TYR B	131	58.554	85.514	1.676	1.00	249.42
	4122 4123	CE2 CZ	TYR B TYR B	131 131	58.929 58.629	85.544 86.660	0.355	1.00	249.42
70	4124	OH	TYP. B	131	58.628 58.902	86.660 86.675	-0.404 -1.726	1.00 1.00	249.42 249.42
							, 20	1.00	£40.42

	4405	•	T/D D				4		
	4125	Ç ·	TYR B	131	55.619	84.751	3.231	1.00	97.57
	4126	0	TYR B	131	54.661	84.439	2.509	1.00	97.57
	4127	N	GLU B	132	56.517	83.862	3.669	1.00	249.33
5	4128 4129	· CB	GLU B	132	56.333	82.428	3.432	1.00	249.33
9	4130	CG	GLU B	132 132	57.528	81.602	3.941	1.00	249.46
	4131	CD	GLU B	132	58.788 59.162	81.623	3.066	1.00	249.46
	4132	OE1	GLU B	132	58.693	80.239 79.231	2.532 3.102	1.00	249.46
	4133	OE2	GLU B	132	59.935	80.161	1.551	1.00	249.46
10	4134	C	GLU B	132	55.158	82.276	4.384	1.00	249.46
10	4135	ŏ	GLU B	132	55.259	82.685	5.543	1.00	249.33
	4136	Ň	ASN B	133	54.047	81.711	3.924	1.00 1.00	249.33
	4137	CA	ASN B	133	52.884	81.642	4.798	1.00	134,43
	4138	CB	ASN B	133	51.649	81.176	4.033	1.00	134.43
15	4139	CG	ASN B	133	51.534	79.690	3.981	1.00	135,42 135,42
	4140	OD1	ASN B	133	52.489	78.995	3.617	1.00	135.42
	4141	ND2	ASN B	133	50.358	79.176	4.337	1.00	135.42
	4142	С	ASN B	133	53.019	80.848	6.080	1.00	134.43
	4143	0	ASN B	133	54.026	80.185	6.338	1.00	134.43
20	4144	N	HIS B	134	51.962	80.932	6.875	1.00	135.01
	4145	CA	HIS B	134	51.905	80.302	8.174	1.00	135.01
	4146	CB	HIS B	134	52.150	81.381	9.224	1.00	225.09
	4147	CG	HIS B	134	52.262	80.865	10.622	1.00	225.09
~~	4148	CD2	HIS B	134	51.493	81.086	11.714	1.00	225.09
25	4149	ND1	HIS B	134	53.283	80.038	11.032	1.00	225.09
	4150	CE1	HIS B	134	53.140	79.772	12.320	1.00	225.09
	4151	NE2	HIS B	134	52.063	80.396	12.756	1.00	225.09
	4152	Ç	HIS B	134	50.531	79.673	8.355	1.00	135.01
20	4153	0	HIS B	134	49.789	79.494	7.385	1.00	135.01
30	4154	N	ASN B	135	50.197	79.346	9.601	1.00	105.44
	4155	CA	ASN B	135	48.928	78. 7 30	9.922	1.00	105.44
	4156	CB	ASN B	135	49.090	77.209	10.001	1.00	235.21
	4157	CG	ASN B	135	49.415	76.600	8.653	1.00	235.21
35	4158 4159	OD1 ND2	ASN B	135	48.779	76.948	7.657	1.00	235.21
55	4160	C	ASN B ASN B	135 135	50.383	75.689	8.604	1.00	235.21
	4161	ŏ	ASN B	135	48.399	79.280	11.223	1.00	105.44
	4162	Ň	ILE B	136	48.611 47.718	78.700 80.417	12 <i>.2</i> 79 11.134	1.00	105.44
	4163	CA	ILE B	136	47.123	81.076	12.304	1.00	66.02
40	4164	CB	ILE B	136	46.015	82.066	11.860	1.00 1.00	66.02
	4165	CG2	ILE B	136	45.045	81.385	10.926	1.00	141.15 141.15
	4166	CG1	ILE B	136	45.283	82.620	13.068	1.00	141.15
	4167	CD1	ILE B	136	44.290	83.673	12.695	1.00	141.15
	4168	С	ILE B	136	46.555	80.069	13.307	1.00	66.02
45	4169	0	ILE B	136	45.602	79.339	13.022	1.00	66.02
	4170	N	SER B	137	47.160	80.045	14.486	1.00	95.21
	4171	CA	SER B	137	46.768	79.114	15.538	1.00	95.21
	4172	CB	SER B	137	47.968	78.233	15.897	1.00	97.51
50	4173	OG	SER B	137	47.742	77.531	17.105	1.00	97.51
50	4174	C	SER B	137	46.218	79.776	16.807	1.00	95.21
	4175	0	SER B	137	46.625	80.869	17.185	1.00	95.21
	4176	N OA	ILE B	138	45.298	79.095	17.472	1.00	236.44
	4177	CA	ILE B	138	44.698	79.625	18.688	1.00	236.44
55	4178	CB	ILE B	138	43.295	80.153	18.420	1.00	113.67
55	4179 4180	CG? CG1	ILE B	138	42.601	80.445	19.737	1.00	113.67
	4181	CD1	ILE B	138	43.363	81.397	17.533	1.00	113.67
	4182	C	ILE B	138	42.021	81.787	16.948	1.00	113.67
	4183	ŏ	ILE B	138 138	44.580	78.558 77.531	19.761	1.00	236.44
60	4184	Ň	THR B	139	43.936 45.180	77.531 78.816	19.555	1.00	236.44
	4185	CA	THR B	139	45.131	77.865	20.915 22.018	1.00	117.60
	4186	CB	THR B	139	46.259	78.143	23.020	1.00 1.00	117.60 212.12
	4187	OG1	THR B	139	46.227	79.521	23.406	1.00	212.12
	4188	CG2	THR B	139	47.609	77.830	22.390	1.00	212.12
65	4189	C	THR B	139	43.780	77.942	22.733	1.00	117.60
	4190	Ō	THR B	139	42.898	77.092	22.541	1.00	117.60
	4191	N	ASN B	140	43.633	78.960	23.573	1.00	147.27
	4192	CA	ASN B	140	42.396	79.189	24.308	1.00	147.27
70	4193	СВ	ASN B	140	42.685	79.890	25.631	1.00	247.00
70	4194	CG	ASN B	140	41.426	80.263	26.369	1.00	247.00
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	4195	OD1	ASN B	140	40,498	80.833	25.789	1.00	
	4196	ND2	ASN B	140	41.395	79.951	25.769 27.658	1.00 1.00	247.00
	4197	С	ASN B	140	41.572	80.103	23.421	1.00	247.00 147.27
_	4198	Ο.	ASN B	140	42.004	81.206	23.092	1.00	147.27
5	4199	N	ALA B	141	40.383	79.652	23.048	1.00	102.95
	4200 4201	CA CB	ALA B	141	39.537	80.432	22.163	1.00	102.95
	4202	C	ALA B	141 141	38.862	79.519	21.162	1.00	101.29
	4203	ŏ	ALA B	141	38.493 37.722	81.273 80.782	22.850 23.680	1.00	102.95
10	4204	Ň	THR B	142	38.458	82.546	22.474	1.00 1.00	102.95
	4205	CA	THR B	142	37.495	83.478	23.021	1.00	139.44 139.44
	4206	CB	THR B	142	38.055	84.903	22.959	1.00	140.37
	4207	OG1	THR B	142	39.366	84.918	23.544	1.00	140.37
15	4208 4209	CG2 C	THR B	142	37.166	85.858	23.725	1.00	140.37
13	4210	Ö	THR B	142 142	36.220 36.216	83.361	22.184	1.00	139.44
	4211	Ň	VAL B	143	35.132	82.675 83.988	21.160 22.623	1.00 1.00	139.44
	4212	CA	VAL B	143	33.884	83.922	21.866	1.00	168.09 168.09
	4213	∪B	VAL B	143	32.633	84.134	22.755	1.00	243.26
20	4214	CG1	VAL B	143	32.616	85.552	23.305	1.00	243.26
	4215	CG2	VAL B	143	31.366	83.867	21.946	1.00	243.26
	4216 4217	C O	VAL B	143	33.925	85.029	20.834	1.00	168.09
	4218	N	GLU B	143 144	33.150 34.839	85.035 85.971	19.878	. 1.00	168.09
25	4219	ĊA	GLU B	144	34.975	87.081	21.035 20.108	1.00 1.00	126.58
	4220	СВ	GLU B	144	35.750	88.229	20.751	1.00	126.58 249.26
	4221	CG	GLU B	144	35.040	88.850	21.940	1.00	249.26
	4222	CD	GLU B	144	35.771	88.603	23.243	1.00	249.26
30	4223 4224	OE1 OE2	GLU B	144	36.942	89.024	23.353	1.00	249.26
50	4225	C	GLU B	144 144	35.181 35.673	87.989	24.157	1.00	249.26
	4226	ŏ	GLU B	144	35.633	86.623 87.305	18.840 17.826	1.00 1.00	126.58
	4227	N	ASP B	145	36.307	85.457	18.903	1.00	126.58 80.30
25	4228	CA	ASP B	145	36.997	84.893	17.752	1.00	80.30
35	4229	СВ	ASP B	145	37.911	83.753	18.189	1.00	204.44
	4230 4231	CG OD1	ASP B	145	39.132	84.250	18.918	1.00	204.44
	4232	OD2	ASP B	145 145	39.896 39.326	85.030	18.310	1.00	204.44
	4233	C	ASP B	145	36.026	83.869 84.395	20.092 16.699	1.00 1.00	204.44
40	4234	0	ASP B	145	36.421	84.133	15.569	1.00	80.30 80.30
	4235	N	SER B	146	34.755	84.263	17.062	1.00	110.67
	4236	CA	SER B	146	33.761	83.800	16.108	1.00	110.67
	4237 4238	CB OG	SER B	146	32.421	83.569	16.815	1.00	166.23
45	4239	c	SER B	146 146	32.547 33.646	82.573 84.870	17.814	1.00	166.23
	4240	ŏ	SER B	146	33.736	86.063	15.022 15.302	1.00 1.00	110.67 110.67
	4241	N	GLY B	147	33.487	84.436	13.778	1.00	85.62
	4242	CA	GLY B	147	33.375	85.365	12.670	1.00	85.62
50	4243	C	GLY B	147	33.473	84.635	11.353	1.00	85.62
50	4244 4245	0 N	GLY B	147	33.311	83.417	11.301	1.00	85.62
	4246	CA	THR B	148 148	33.737 33.851	85.372	10.279	1.00	63.43
	4247	CB	THR B	148	32.729	84.756 85 244	8.952 7.5.41	1.00	63.43
	4248	OG1	THR B	148	33.253	85.244 86.223	7.5 (1 7.403	1.00 1.00	111.42 111.42
55	4249	CG2	THR I	148	31.609	85.879	8.767	1.00	111.42
	4250	C	THR B	148	35.227	85.092	8.397	1.00	63.43
	4251 4252	0	THR B	148	35.568	86.244	8.176	1.00	63.43
	4253	CA	TYR B TYR B	149 149	36.024 37.366	84.069	8.183	1.00	61.50
60	4254	CB	TYR B	149	38.298	84.273 83.380	7.705 8.514	1.00	61.50
	4255	CG	TYR B	149	38.353	83.629	10.007	1.00 1.00	61.70 61.70
	4256	CD1	TYR B	149	37.273	83.361	10.839	1.00	61.70
	4257	CE1	TYR B	149	37.373	83.572	12.217	1.00	61.70
65	4258	CD2	TYR B	149	39.514	84.106	10.587	1.00	61.70
J.J	4259 4260	CE2 CZ	TYR B	149	39.626	84.317	11.939	1.00	61.70
	4261	OH	TYR B	149 149	38.571 38.744	84.060 84.337	12.757	1.00	61.70
	4262	Č.	TYR B	149	37.540	84.327 83.934	14.104 6.223	1.00 1.00	61.70
70	4263	0	TYR B	149	36.666	83.307	5.605	1.00	61.50 61.50
70	4264	N	TYR B	150	38.674	84.372	5.669	1.00	57.66
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	4265	CA	TYR E	150	39.090	84.071	4.302	1.00	57.66
	4266	CB	TYR E	150	38.189	84.760	3.264	1.00	
	4267	CG	TYR E		38.386	86.234	3.018		101.41
	4268	CD1	TYR E					1.00	101.41
5					39.493	86.704	2.338	1.00	101.41
J	4269	CE1	TYR E		39.653	88.065	2.074	1.00	101.41
	4270	CD2	TYR E	150	37.435	87.160	3.428	1.00	101.41
	4271	CE2	TYR E	150	37.582	88.520	3.163	1.00	
	4272	· CZ	TYR E		38.693	88.967			101.41
	4273	OH					2.489	1.00	. 101.41
10					38.855	90.316	2.245	1.00	101.41
10	4274	С	TYR E	150	40.539	84.536	4.251	1.00	57.66
	4275	0	TYR E	150	40.952	85.331	5.109	1.00	57.66
	4276	N	CYS E	151	41,340	84.020	3.318	1.00	
	4277	CA	CYS E		42.736				78.79
	4278	Č				84.458	3.227	1.00	78.79
15			CYS E		43.124	84.856	1.804	1.00	78.79
15	4279	0	CYS E		42.464	84.461	0.849	1.00	78.79
	4280	CB	CYS E	151	43.680	83.369	3.736	1.00	103.97
	4281	SG	CYS E	151	43.510	81.730	2.951	1.00	
	4282	N	THR E						103.97
	4283				44.174	85.668	1.673	1.00	109.05
20		CA	THR E		44.663	86.107	0.370	1.00	109.05
20	4284	CB	THR B		44.524	87.630	0.206	1.00	169.15
	4285	OG1	THR B	152	45.394	88.296	1.133	1.00	169.15
	4286	CG2	THR B	152	43.097	88.056	0.475	1.00	
	4287	С	THR B		46.139	85.728			169.15
	4288	ŏ	THR B				0.297	1.00	109.05
25					46.839	85.740	1.317	1.00	109.05
23	4289	N	GLY B		46.611	85.381	-0.898	1.00	135.93
	4290	CA	GLY B	153	48.007	85.000	-1.054	1.00	135.93
	4291	С	GLY B	153	48.447	85.023	-2.501	1.00	
	4292	0	GLY B	153	47.618	85.025	-3.404		135.93
	4293	Ň	LYS B					1.00	135.93
30					49.751	85.038	-2.734	1.00	88.42
30	4294	CA	LYS B		50.252	85.068	-4.096	1.00	88.42
	4295	CB	LYS B	154	51.392	86.090	-4.216	1.00	187.09
	4296	CG	LYS B	154	51.920	86.317	-5.630	1.00	187.09
	4297	CD	LYS B		53.003	87.393	-5.619	1.00	
	4298	CE	LYS B						187.09
35	4299	NZ			53.634	87.579	-6.975	1.00	187.09
55			LYS B		54.766	88.490	-6.839	1.00	187.09
	4300	Ç	LYS B		50.744	83.673	-4.404	1.00	88.42
	4301	0	LYS B		51.450	83.057	-3.592	1.00	88.42
	4302	N	VAL B	155	50.332	83.166	-5.561	1.00	135.91
	4303	CA	VAL B		50.742	81.845	-6.018	1.00	
40	4304	CB	VAL B		49.550				135.91
	4305	CG1				80.923	-6.254	1.00	118.28
			VAL B		50.030	79.574	-6.748	1.00	118.28
	4306	CG2	VAL B		48.773	80.767	-4.968	1.00	118.28
	4307	С	VAL B	155	51.459	82.067	-7.332	1.00	135.91
	4308	0	VAL B	155	50.938	82.731	-8.237	1.00	135.91
45	4309	N	TRP B		52.655	81.505			
	4310	CA	TRP B				-7.433	1.00	121.66
					53.453	81.702	-8.624	1.00	121.66
	4311	СВ	TRP B		52.679	81.359	-9.884	1.00	200.98
	4312	CG	TRP B		52.385	79.963	-9.953	1.00	200.98
	4313	CD2	TRP B	156	53.333	78.905	-9.901	1.00	200.98
50	4314	CE2	TRP B		52.609	77.699			
	4315	CE3	TRP B				-9.939	1.00	200.98
	4316				54.730	78.860	-9.823	1.00	200.98
		CD1	TRP B		51.160	79.393	-10.027	1.00	200.98
	4317	NE1	TRP B		51.283	78.024	-10.013	1.00	200.98
	4318	CZ2	TRP B	156	53.232	76.454	-9.905	1.00	200.98
55	4319	CZ3	TRP B		55.352	77.622			
	4320	CH2	TRP B	156			-9.790	1.00	200.98
					54.59 թ	76.432	-9.834	1.00	200.98
	4321	C	TRP B		53.739	83.168	-8.671	1.00	121.66
	4322	0	TRP B	156	54.677	83.647	-8.029	1.00	121.66
	4323	N	GLN B	157	52.883	83.878	-9.403	1.00	111.84
60	4324	CA	GLN B		53.057	85.297	-9.568		
	4325	CB	GLN B					1.00	111.84
	4326	CG			53.912	85.525	-10.808	1.00	249.48
			GLN B		55.364	85.155	-10.531	1.00	249.48
	4327	CD	GLN B		55.818	85.806	-9.260	1.00	249.48
	4328	OE1	GLN B	157	55.599	86.983	-9.081	1.00	249.48
65	4329	NE2	GLN B		56.437	85.047	-8.360	1.00	
	4330	C	GLN B		51.781				249.48
	4331	ŏ				86.092	-9.614	1.00	111.84
			GLN B	157	51.785	87.265	-9.988	1.00	111.84
	4332	N	LEU B		50.688	85.447	-9.217	1.00	140.68
70	4333	CA	LEU B	158	49.392	86.104	-9.195	1.00	140.68
70	4334	CB	LEU B		48.463	85.512	-10.253	1.00	
								1.00	225.85

	4335	CG	LEV B	158	48.673	85.926	-11.710	1.00	225.85
	4336 4337	CD1 CD2:	LEV B LEV B	158	47.296	86.093	-12.325	1.00	225.85
	4337	CU2 ⁻ .	LEU B	158	49.447	87.239	-11.827	1.00	225.85
5	4339	ŏ	LEU B	158 158	48.724 48.980	86.035 85.125	-7. 829 -7.039	1.00	140.68
•	4340	Ň	ASP B	159	47.870	87.017	-7.560	1.00 1.00	140.68
	4341	CA	ASP B	159	47.162	87.101	-6.291	1.00	142.12 142.12
	4342	CB	ASP B	159	46.879	88.574	-5.943	1.00	249.27
	4343	CG	ASP B	159	48.138	89.443	-5.949	1.00	249.27
10	4344	OD1	ASP B	159	49.066	89.181	-5.152	1.00	249.27
	4345	OD2	ASP B	159	48.194	90.399	-6.754	1.00	249.27
	4346 4347	C	ASP B ASP B	159	45.846	86.325	-6.363	1.00	142.12
	4348	0 N	ASP B TYR B	159 160	45.204	86.280	-7.414	1.00	142.12
15	4349	CA	TYR B	160	45.456 44.209	85.711 84.946	-5.244 -5.164	1.00 1.00	173.61
	4350	CB	TYR B	160	44.442	83.463	-5.430	1.00	173.61 249.32
	4351	CG	TYR B	160	45.173	83.176	-6.709	1.00	249.32
	4352	CD1	TYR B	160	46.561	83.098	-6.731	1.00	249.32
20	4353	CE1	TYR B	160	47.246	82.846	-7.908	1.00	249.32
20	4354 4355	CD2 CE2	TYR B	160	44.481	82.995	-7.903	1.00	249.32
	4356	CZ	TYR B TYR B	160 160	45.155	82.744	-9.091	1.00	249.32
	4357	OH	TYR B	160	46.540 47.221	82.671 82.428	-9.085 -10.254	1.00 1.00	249.32
	4358	C	TYR B	160	43.517	85.072	-3.818	1.00	249.32 173.61
25	4359	0	TYR B	160	44.155	85.185	-2.768	1.00	173.61
	4360	N	GLU B	161	42.194	85.014	-3.871	1.00	90.61
	4361	CA	GLU B	161	41.341	85.130	-2.695	1.00	90.61
	4362	CB	GLU B	161	40.333	86.257	-2.926	1.00	219.32
30	4363 4364	CD	GLU B	161	39.312	86.469	-1.834	1.00	219.32
50	4365	OE1	GLU B	161 161	38.626 37.530	87.808 87.986	-1.980 -1.409	1.00 1.00	219.32
	4366	OE2	GLU B	161	39.197	88.688	-2.663	1.00	219.32 219.32
	4367	С	GLU B	161	40.634	83.792	-2.513	1.00	90.61
25	4368	0	GLU B	161	40.215	. 83,179	-3.486	1.00	90.61
35	4369	N	SER B	162	40.522	83.335	-1.270	1.00	91.35
	4370 4371	CA CB	SER B	162	39.884	82.057	-0.957	1.00	91.35
	4372	OG	SER B SER B	162 162	40.575 40.507	81.414 82.266	0.251	1.00	56.32
	4373	Č	SER B	162	38.401	82.220 82.220	1.391 -0.664	1.00 1.00	56.32 91.35
40	4374	Ŏ	SER B	162	37.909	83.344	-0.522	1.00	91.35
	4375	N	GLU B	163	37.690	81.097	-0.574	1.00	79.84
	4376	CA	GLU B	163	36.253	81.114	-0.287	1.00	79.84
	4377	CB	GLU B	163	35.639	79.737	-0.529	1.00	200.03
45	4378 4379	CG CD	GLU B GL!; B	163 163	35.475	79.360	-1.993	1.00	200.03
	4380	OE1	GLU B	163	34.355 33.206	80.127 80.054	-2.674 -2.187	1.00 1.00	200.03
	4381	QE2	GLU B	163	34.621	80.795	-3.698	1.00	200.03 200.03
	4382	С	GLU B	163	36.094	81.500	1.169	1.00	79.84
50	4383	0	GLU B	163	36.886	81.075	1.996	1.00	79.84
30	4384	N	PRO B	164	35.068	82.315	1.508	1.00	60.77
	4385 4386	CD CA	PRO B	164	34.003	82.898	0.682	1.00	73.97
	4387	CB	PRO B PRO B	164 164	34.904 33.877	82.700 83.829	2.920	1.00	60.77
	4388	ČG	PRO B	164	33.008	83.388	2.847 1.730	1.00 1.00	73.97
55	4389	C	PRO B	164	34.431	81.530	3.744	1.00	73.97 60.77
	4390	0	PRO B	164	33.842	80.588	3.223	1.00	6°.77
	4391	N	LEU B	165	34.700	81.568	5.035	1.00	63.41
	4392	CA	LEU B	165	34.288	80.472	5.889	1.00	63.41
60	4393 4394	CB CG	LEU B LEU B	165	35.440	79.499	6.070	1.00	68.59
00	4395	CD1	LEU B	165 165	35.185 33.824	78.450 77.858	7.138	1.00	68.59
	4396	CD2	LEU B	165	38.264	77.380	6.851 7.140	1.00 1.00	68.59 68.59
	4397	С	LEU B	165	33.847	80.963	7.250	1.00	63.41
CF	4398	0	LEU B	165	34.613	81.635	7.953	1.00	63.41
65	4399	N	, ASN B	166	32.623	80.613	7.628	1.00	64.97
	4400	CA	ASN B	166	32.078	81.041	8.911	1.00	64.97
	4401 4402	CB CG	ASN B	166	30.556	81.011	8.900	1.00	96.05
	4403	OD1	ASN B ASN B	166 166	29.945 30.504	82.338	8.491	1.00	96.05
70	4404	ND2	ASN B	166	28.773	83.403 82.270	8.737 7.884	1.00 1.00	96.05
		· 				V / V	7.004	1.00	96.05

	4405	С	ASN B	166	32.556	80.174	10.040	1.00	64.07
	4406	0	ASN B	166	32.754	78.988	9.860	1.00	64.97
	4407	N .	ILE B	167	32.720	80.766	11.213	1.00	64.97
_	4408	CA	ILE B	167	33.183	80.034	12.375	1.00	77.41 77.41
5	4409	CB	ILE B	167	34.653	80.263	12.591	1.00	59.98
	4410	CG2	ILE B	167	35.050	79.859	13.985	1.00	59.98
	4411	CG1	ILE B	167	35.434	79.484	11.546	1.00	59.98
	4412	CD1	ILE B	167	36.942	79.537	11.784	1.00	59.98
10	4413	Ç	ILE B	167	32.467	80.488	13.622	1.00	77.41
10	4414	0	ILE B	167	32,375	81.676	13.896	1.00	77.41
	4415	N	THR B	168	31.972	79.548	14.405	1.00	104.04
	4416	CA	THR B	168	31.283	79.938	15.610	1.00	104.04
	4417	CB	THR B	168	29.817	79.572	15.536	1.00	107.45
15	4418 4419	OG1 CG2	THR B	168	29.239	80.179	14.374	1.00	107.45
15	4420	CGZ	THR B	168	29.096	80.067	16.766	1.00	107.45
	4421	ŏ	THR B	168 168	31.888	79.326	16.850	1.00	104.04
	4422	Ň	VAL B	169	32.254 32.012	78.155	16.886	1.00	104.04
	4423	ČA	VAL B	169	32.544	80.155 79.737	17.867	1.00	108.46
20	4424	CB	VAL B	169	33.748	80.618	19.146 19.5 6 3	1.00	108.46
-	4425	CG1	VAL B	169	33.974	80.539	21.049	1.00 1.00	68.82
	4426	CG2	VAL B	169	34.981	80.174	18.834	1.00	68.82
•	4427	C	VAL B	169	31.394	79.942	20.129	1.00	68.82
	4428	0	VAL B	169	31.047	81.082	20.455	1.00	108.46 108.46
25	4429	N	ILE B	170	30.790	78.844	20.579	1.00	128.18
	4430	CA	ILE B	170	29.679	78.917	21.525	1.00	128.18
	4431	CB	ILE B	170	28.680	77.760	21.285	1.00	141.23
	4432	CG2	ILE B	170	28.276	77.749	19.833	1.00	141.23
20	4433	CG1	ILE B	170	29.321	76.414	21.631	1.00	141.23
30	4434	CD1	ILE B	170	28.423	75.218	21.463	1.00	141.23
	4435	Ç	ILE B	170	30.228	78.854	22.946	1.00	128.18
	4436	0	ILE B	170	31.426	78.679	23.142	1.00	128.18
	4437	N	LYS B	171	29.365	79.005	23.941	1.00	164.76
35	4438	CA	LYS B	171	29.816	78.956	25.328	1.00	164.76
33	4439	CB	LYS B	171	29.779	80.358	25.929	1.00	211.84
	4440 4441	CG	LYS B	171	28.416	81.020	25.858	1.00	211.84
	4442	CD CE	LYS B	171	28.536	82.537	25.911	1.00	211.84
	4443	NZ	LYS B	171	29.207	83.011	27.190	1.00	211.84
40	4444	C	LYS B	171 171	29.341 28.987	84.494	27.217	1.00	211.84
	4445	ŏ	LYS B	171	29.329	77.998 77.724	26.180	1.00	164.76
	4446	Č1	NAG B	221	47.345	59.956	27.330	1.00	164.76
	4447	C2	NAG B	221	48.521	60.923	-1.693 -1.796	1.00 1.00	249.77
	4448	N2	NAG B	221	48.022	62.275	-1.936	1.00	249.77
45	4449	C7	NAG B	221	48.763	63.299	-1.535	1.00	249.77 249.77
	4450	07	NAG B	221	49.873	63.160	-1.022	1.00	249.77
	4451	C8	NAG B	221	48.181	64.690	-1.724	1.00	249.77
	4452	СЗ	NAG B	221	49.387	60.591	-3.002	1.00	249.77
50	4453	O3	NAG B	221	50.560	61.387	-2.974	1.00	249.77
50	4454	C4	NAG B	221	49.783	59.115	-3.044	1.00	249.77
	4455	04	NAG B	221	50.388	58.867	-4.330	1.00	249.77
	4456	C5	NAG B	221	48.535	58.221	-2.850	1.00	249.77
	4457	O5	NAG B	221	47.825	58.605	-1.651	1.00	249.77
55	4458	C6	NAG B	221	48.869	56.745	-2.696	1.00	249.77
55	4459 4460	O6	NAG B	221	49.689	56.518	-1.557	1.00	249.77
	4461	C1 C2	NAG B	222	51.148	57.718	-4.505	1.00	249.77
	4462	N2	NAG B	222	52.440	58.058	-5.267	1.00	249.77
	4463	C7	NAG B	222	53.222	59.027	-4.521	1.00	249.77
60	4464	O7	NAG B NAG B	222 222	54.445	58.717	-4.103	1.00	249.77
	4465	C8	NAG B	222	54.970 55.100	57.622 50.786	-4.314 2.222	1.00	249.77
	4466	Čŝ	NAG B	222	55.199 52.103	59.786 59.614	-3.332	1.00	249.77
	4467	03	NAG B	222	53.301	58.614 58.775	-6.661 -7.409	1.00	249.77
	4468	C4	NAG B	222	51.148	57.668	-7.409 -7.412	1.00	249.77
65	4469	04	NAG B	222	50.712	58.282	-7.412 -8.619	1.00 1.00	249.77 249.77
	4470	C5	NAG B	222	49.930	57.333	-6.541	1.00	249.77 249.77
	4471	O5	NAG B	222	50.362	56.787	·5.270	1.00	249.77 249.77
	4472	C6	NAG B	222	49.003	56.316	-7.180	1.00	249.77
70	4473	O 6	NAG B	222	47.646	56.720	-7.068	1.00	249.77
70	4474	C1	NAG B	242	26.466	62.870	-0.923	1.00	89.47
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	4475	C2	NAG B	242 -	26.972	62.476	-2.293	1.00	89.47
	4476	N2	NAG B	242	27.712	61.243	-2.203	1.00	89.47
	4477	C7	NAG B	242	27.358	60.216	-2.956	1.00	89.47
_	4478	07	NAG B	242	26.416	60.270	-3.732	1.00	89.47
5	4479	C8	NAG B	242	28.159	58.938	-2.829	1.00	89.47
	4480	C3	NAG B	242	27.882	63.561	-2.855	1.00	89.47
	4481	O 3	NAG B	242	28.253	53.234	-4.180	1.00	89.47
	4482	C4	NAG B	242	27.180	64.901	-2.854	1.00	89.47
	4483	O4	NAG B	242	28.116	65.947	-3.186	1.00	89.47
10	4484	C5	NAG B	242	26.567	65.197	-1.493	1.00	89.47
	4485	O 5	NAG B	242	25.753	64.083	-1.046	1.00	89.47
	4486	C6	NAG B	242	25.657	66.413	-1.634	1.00	89.47
	4487	O6	NAG B	242	25.965	67.439).691	1.00	89.47
	4488	C1	NAG B	243	27.860	66.616	363	1.00	124.06
15	4489	C2	NAG B	243	28.444	68.031	-4.311	1.00	124.06
	4490	N2	NAG B	243	27.812	68.814	-3.263	1.00	124.06
	4491	C7	NAG B	243	28.560	69.543	-2.441	1.00	124.06
	4492	07	NAG B	243	29.786	69.568	-2.502	1.00	124.06
00	4493	C8	NAG B	243	27.853	70.353	-1.378	1.00	124.06
20	4494	C3	NAG B	243	28.214	63.724	-5.658	1.00	124.06
	4495	O 3	NAG B	243	28.825	70.012	-5.653	1.00	124.06
	4496	C4	NAG B	243	28.765	67.860	-6.816	1.00	124.06
	4497	04	NAG B	243	28.392	68.459	-8.089	1.00	124.06
0.5	4498	C5	NAG B	243	28.162	6o.455	-6.717	1.00	124.06
25	4499	O5	NAG B	243	28.449	65.870	-5.432	1.00	124.06
	4500	C6	NAG B	243	28.638	65.499	-7.762	1.00	124.06
	4501	O 6	NAG B	243	30.003	65.214	-7.571	1.00	124.06
	4502	C1	MAN B	244	29.308	68.650	-9.080	1.00	182.20
20	4503	C2	MAN B	244	30.527	69.553	-8.800	1.00	182.20
30	4504	02	MAN B	244	31.636	68.751	-8.489	1.00	182.20
	4505	C3	MAN B	244	30.736	70.260	-10.177	1.00	182.20
	4506	03	MAN B	244	31.834	71.153	-10.165	1.00	182.20
	4507	C4	MAN B	244	30.850	69.264	-11.367	1.00	182.20
35	4508	04	MAN B	244	31.059	69.973	-12.588	1.00	182.20
33	4509	C5	MAN B	244	29.519	68.480	-11.433	1.00	182.20
	4510	O5	MAN B	244	29.290	67.732	-10.210	1.00	182.20
	4511	C6	MAN B	244	29.376	67.561	-12.650	1.00	182.20
	4512	O6 C1	MAN B	244	30.030	66.327	-12.454	1.00	182.20
40	4513 4514	C2 .	NAG B	250	42.367	49.115	8.367	1.00	249.70
40	4515	N2	NAG B NAG B	250	43.729	49.074	9.087	1.00	249.70
	4516	C7	NAG B	250	43.544	49.049	10.526	1.00	249.70
	4517	07	NAG B	250 250	43.853	47.960	11.227	1.00	249.70
	4518	C8	NAG B	250 250	44.295 43.632	46.930	10.709	1.00	249.70
45	4519	C3	NAG B	250 250	43.632 44.545	48.021 50.311	12.734	1.00	249.70
	4520	O3	NAG B	250	45.842	50.245	8.692	1.00	249.70
	4521	Č4	NAG B	250	44.660	50.407	9.269 7.167	1.00	249.70
	4522	04	NAG B	250	45.304	51.625	6.813	1.00 1.00	249.70
	4523	C5	NAG B	250	43.262	50.349	6.521	1.00	249.70
50	4524	O5	NAG B	250	42.562	49.158	6.946	1.00	249.70 249.70
	4525	C6	NAG B	250	43.315	50.314	5.003	1.00	
	4526	06	NAG B	250	42.060	49.940	4,449	1.00	249.70
	4527	C1	NAG B	274	20.954	54.260	22.053	1.00	249.70
	4528	C2	NAG B	274	20.822	55.380	23.099	1.00	246.89
55	4529	N2	NAG B	274	21.918	55.314	24.050	1.00	246.89 246 99
	4530	C7	NAG B	274	22.298	56.407	24.706	1.00	
	4531	07	NAG B	274	21.767	57. 5 06	24.541	1.00	246.89 246.89
	4532	C8	NAG B	274	23.446	56.263	25.690	1.00	246.89
_	4533	C3	NAG B	274	19.484	55.246	23.844	1.00	246.89
60	4534	O3	NAG B	274	19.302	56.360	24.707	1.00	246.89
	4535	C4	NAG B	274	18.314	55.163	22.856	1.00	246.89
	4536	04	NAG B	274	17.111	54.887	23.563	1.00	246.89
	4537	C5	NAG B	274	18.576	54.059	21.820	1.00	246.89
	4538	O5	NAG B	274	19.837	54.291	21.151	1.00	246.89
65	4539	C6	NAG B	274	17.507	53.987	20.743	1.00	246.89
	4540	O6	NAG B	274	17.896	53.120	19.688	1.00	246.89
	4541	C1	NAG B	335	50.085	74.386	8.041	1.00	247.49
	4542	C2	NAG B	335	50.430	73.230	9.006	1.00	247.49
70	4543	N2	NAG B	335	50.451	73.760	10.357	1.00	247.49
70	4544	C7	NAG B	335	49.583	73.330	11.267	1.00	247.49

	4545	07	NAG B	335	48.734	72.471	11.036	1.00	247.49
	4546 4547	C8 ⇔	NAG B	335	49.680	73.947	12.649	1.00	247.49
	4548	C3 O3	NAG B NAG B	335 335	51.781	72.552	8.725	1.00	247.49
5	4549	Č4	NAG B	335	51.808 52.016	71.282 72.369	9.359	1.00	247.49
	4550	04	NAG B	335	53.304	71.813	7.231 7.004	1.00 1.00	247.49
	4551	C5	NAG B	335	51.906	73.729	6.561	1.00	247.49
	4552	O5	NAG B	335	50.550	74.212	6.679	1.00	247.49 247.49
10	4553	C6	NAG B	335	52.229	73.654	5.078	1.00	247.49
10	4554	O6	NAG B	335	53.343	74.471	4.748	1.00	247.49
	4555 4556	C1 C2	NAG B NAG B	340	41.414	81.009	28.648	1.00	249.67
	4557	N2	NAG B	340 340	40.114 38.971	80.981	29.434	1.00	249.67
	4558	C7	NAG B	340	37.997	81.033 80.133	28.539 28.666	1.00 1.00	249.67
15	4559	O 7	NAG B	340	38.012	79.245	29.526	1.00	249.67 249.67
	4560	C8	NAG B	340	36.831	80.226	27.702	1.00	249.67
	4561	cs	NAG B	340	40.092	82.143	30.420	1.00	249.67
	4562 4563	O3	NAG B	340	38.904	82.071	31.207	1.00	249.67
20	4564	C4 O4	NAG B NAG B	340 340	41.329 41.393	82.067	31.330	1.00	249.67
	4565	C5	NAG B	340	42.643	83.255 81.894	32.105	1.00	249.67
	4566	O5	NAG B	340	42.519	80.841	30.520 29.539	1.00 1.00	249.67
	4567	C6	NAG B	340	43.832	81.515	31.388	1.00	249.67 249.67
25	4568	O6	NAG B	340	44.745	80.677	30.696	1.00	249.67
25	4569	C1	NAG B	366	28.147	83.475	7.400	1.00	133.05
	4570	C2	NAG B	366	27.352	83.132	6.154	1.00	133.05
	4571 4572	N2 C7	NAG B NAG B	366	28.247	82.591	5.149	1.00	133.05
	4573	07 07	NAG B	366 366	28.452 27.909	81.278	5.075	1.00	133.05
30	4574	Č8	NAG B	366	29.408	80.467 80.789	5.829 3.998	1.00 1.00	133.05
	4575	СЗ	NAG B	366	26.651	84.373	5.618	1.00	133.05 133.05
	4576	O3	NAG B	366	25.783	84.003	4.553	1.00	133.05
	4577	C4	NAG B	366	25.842	85.068	6.713	1.00	133.05
35	4578 4579	O4 C5	NAG B	366	25.403	86.347	6.211	1.00	133.05
33	4580	O5	NAG B NAG B	366 366	26.688 27.291	85.270	7.986	1.00	133.05
•	4581	C6	NAG B	366	25.864	84.029 85.757	8.400 9.163	1.00	133.05
	4582	O 6	NAG B	366	26.677	85.957	10.310	1.00 1.00	133.05 133.05
40	4583	C1	NAG B	367	24.042	86.610	6.284	1.00	230.72
40	4584	C2	NAG B	367	23.806	88.121	6.264	1.00	230.72
	4585 4586	N2 C7	NAG B	367	24.497	88.757	7.369	1.00	230.72
	4587	07	NAG B NAG B	367 367	25.574	89.501	7.133	1.00	230.72
	4588	C8	NAG B ~		26.030 26.251	89.681 90.141	6.002 8.334	1.00	230.72
45	4589	C3	NAG B	367	22.301	88.392	6.337	1.00 1.00	230.72 230.72
	4590	O3	NAG B	367	22.054	89.791	6.274	1.00	230.72
	4591	C4	NAG B	367	21.604	87.688	5.169	1.00	230.72
	4592	O4	NAG B	367	20.197	87.854	5.276	1.00	230.72
50	4593 4594	C5 O5	NAG B NAG B	367	21.956	86.193	5.170	1.00	230.72
30	4595	C6	NAG B	367 367	23.395 21.396	86.007	5.152	1.00	230.72
	4596	0 6	NAG B	367	22.431	85.477 85.064	3.959 3.078	1.00	230.72
	4597	CB	LYS D	4	55.111	67.727	55.236	1.00	230.72
E E	4598	CG	LYS D	4	54.671	66.297	5.1.972	1.00	220.56 220.56
55	4599	CD	LYS D	4	54.274	65.601	56.262	1.00	220.56
	4600 4601	CE NZ	LYS D	4	53.817	64.172	56.007	1.00	220.56
	4602	C	LYS D LYS D	4 4	53.427	63.496	57.274	1.00	220.56
	4603	ŏ	LYS D	4	54.245 53.112	68.471 68.293	53.028	1.00	175.22
60	4604	N	LYS D	4	55.813	69.908	53.459 54.320	1.00 1.00	175.22 175.22
	4605	CA	LYS D	4	55.442	68.509	53.968	1.00	175.22
	4606	N	PRO D	5	54.485	68.654	51.722	1.00	119.81
	4607	CD	PRO D	5	55.727	69.166	51.125	1.00	90.67
65	4608 4609	CA CB	PRO D	5	53.397	68.631	50.737	1.00	119.81
	4610	CG	PRO D PRO D	5 5	53.950 55.400	69.490	49.602	1.00	90.67
	4811	Č	PRO D	5	53.035	69.182 67.215	49.643 50.281	1.00	90.67
	4612	0	PRO D	5	53.836	66.281	50.281	1.00 1.00	119.81 119.81
70	4613	N	LYS D	6	51.824	67.054	49.752	1.00	96.52
70	4614	CA	LYS D	6	51.373	65.747	49.285	1.00	96.52
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	4615	CB	LYS D	6	50.549	65.060	50.379	1.00	171.50
	4616	CG	LYS D	6	50.141	63.639	50.041		
	4617	CD	LYS D	6	49.490	62.929		1.00	171.50
	4618	CE	LYS D	6			51.225	1.00	171.50
5	4619				49.128	61.483	50.860	1.00	171.50
,		NZ	LYS D	6	48.560	60.707	52.003	1.00	171.50
	4620	Ç	LYS D	6	50.557	65.881	47.994	1.00	96.52
	4621	0	LYS D	6	49.495	66.491	47.981	1.00	96.52
	4622	N	VAL D	7	51.072	65.306	46.911	1.00	68.94
	4623	CA	VAL D	7	50.422	65.353	45.604	1.00	
10	4624	CB	VAL D	7	51.321	64.793			68.94
. •	4625	CG1	VAL D				44.498	1.00	87.54
				7	50.661	65.026	43.147	1.00	87.54
	4626	CG2	VAL D	7	52.693	65.408	44.566	1.00	87.54
	4627	С	VAL D	7	49.159	64.529	45.521	1.00	68.94
	4628	0	VAL D	7	49.213	63.311	45.658	1.00	68.94
15	4629	N	SER D	8	48.033	65.178	45.263	1.00	
	4630	CA	SER D	8	46.766	64.465	45.138		67.77
	4631	CB	SER D	8	45.651			1.00	67.77
	4632	og Og				65.209	45.877	1.00	176.15
			SER D	8	45.554	66.551	45.438	1.00	176.15
20	4633	С	SER D	8	46.434	64.349	43.651	1.00	67.77
20	4634	0	SER D	8	47.041	65.043	42.834	1.00	67.77
	4635	N	LEU D	9	45.500	63.459	43.304	1.00	116.14
	4636	CA	LEU D	9	45.098	63.252	41.912	1.00	
	4637	СВ	LEU D	9	45.531	61.883	41.396		116.14
	4638	CG	LEU D					1.00	98.23
25	4639			9	47.001	61.491	41.352	1.00	98.23
25		CD1	LEU D	9	47.193	60.359	40.372	1.00	98.23
	4640	CD2	LEU D	9	47.818	62.671	40.913	1.00	98.23
	4641	С	LEU D	9	43.596	63.326	41.770	1.00	116.14
	4642	0	LEU D	9	42.865	63.094	42.732	1.00	116.14
	4643	N	ASN D	10	43.135	63.630	40.560	1.00	
30	4644	CA	ASN D	10	41.699	63.718			87.18
	4645	CB	ASN D				40.284	1.00	87.18
				10	41.130	65.052	40.768	1.00	123.83
	4646	CG	ASN D	10	39.625	65.064	40.746	1.00	123.83
	4647	OD1	ASN D	10	38.973	64.342	41.505	1.00	123.83
~ ~	4648	ND2	ASN D	10	39.058	65.867	39.857	1.00	123.83
35	4649	C	ASN D	10	41.419	63.561	38.797	1.00	87.18
	4650	0	ASN D	10	41.732	64.453	38.000	1.00	87.18
	4651	N	PRO D	11	40.804	62.432	38.402	1.00	
	4652	CD	PRO D	11	40.609				137.25
	4653	GA				62.151	36.972	1.00	119.64
40			PRO D	11	40.349	61.301	39.221	1.00	137.25
40	4654	СВ	PRO D	11	39.877	60.298	38.167	1.00	119.64
	4655	CG	PRO D	11	39.503	61.164	37.007	1.00	119.64
	4656	C	PRO D	11	41.422	60.689	40.148	1.00	137.25
	4657	0	PRO D	11	42.614	60.926	39.952	1.00	137.25
	4658	N	PRO D	12	41.017	59.899	41.164	1.00	
45	4659	CD	PRO D	12	39.630				96.57
	4660	CA				59.557	41.534	1.00	83.5
			PRO D	12	41.951	59.269	42.104	1.00	96.57
	4661	СВ	PRO D	12	41.041	58.629	43.151	1.00	83.91
	4662	CG	PRO D	12	39.761	59.344	43.011	1.00	83.91
	4663	С	PRO D	12	42.774	58.205	41.374	1.00	96.57
50	4664	0	PRO D	12	43.874	57.834	41.802	1.00	96.57
	4665	N	TRP D	13	42.222	57.717	40.268	1.00	
	4668	CA	TRP D	13	42.869	56.675	39.486		86.01
	4667	CB	TRP D					1.00	86.01
				13	42.032	56.366	38.247	1.00	97.24
55	466:	CG	TRP D	13	40.601	56.191	38.568	1.00	97.24
23	466∂	CD2	TRP D	13	40.049	55.556	39.724	1.00	97.2
	4670	CE2	TRP D	13	38.651	55.664	39.631	1.00	97.24
	4671	CE3	TRP D	13	40.604	54.902	40.836	1.00	97.24
	4672	CD1	TRP D	13	39.546	56.637	37.836		
	4673	NE1	TRP D	13	38.370			1.00	97.24
60	4674	CZ2	TOO D			56.330	38.469	1.00	97.24
00		022	TRP D	13	37.795	55.147	40.609	1.00	97.24
	4675	CZ3	TRP D	13	39.753	54.387	41.804	1.00	97.24
	4676	CH2	TRP D	13	38.364	54.515	41.686	1.00	97.24
	4677	С	TRP D	13	44.278	57.041	39.075	1.00	86.01
	4678	0	TRP D	13	44.493	58.036	38.401	1.00	86.01
65	4679	Ň	ASN D	14	45.244	56.231	39.488	1.00	79.52
	4680	CA	ASN D	14	46.627				
	4681	CB				56.488	39.122	1.00	79.52
			ASN D	14	47.534	56.449	40.358	1.00	103.31
	4682	CG	ASN D	14	47.664	55.067	40.958	1.00	103.31
70	4683	OD1	ASN D	14	46.871	54.415	41.283	1.00	103.31
70	4684	ND2	ASN D	14	48.895	54.618	41.124	1.00	103.31

	4685	С	ASN D	14	47,153	55.545	38.031	1.00	70.50
	4686	0	ASN D	14	48.358	55.444	37.825	1.00	79.52 79.52
	4687	N	ARG D	15	46.248	54.842	37.351	1.00	78.52 58.96
_	4688	CA	ARG D	15	46.609	53.977	36.231	1.00	58.96
5	4689	СВ	ARG D	15	46.413	52.517	36.552	1.00	70.76
	4690	CG	ARG D	15	46.829	52.131	37.918	1.00	70.76
	4691	CD	ARG D	15	46.633	50.641	38.077	1.00	70.76
	4692	NE	ARG D	15	47.557	49.869	37.263	1.00	70.76
10	4693	CZ	ARG D	15	47.280	48.660	36.802	1.00	70.76
10	4694 4695	NH1 NH2	ARG D	15	46.108	48.121	37.078	1.00	70.76
	4696	C	ARG D ARG D	15 15	48.170	47.981	36.079	1.00	70.76
	4697	ŏ	ARG D	15	45.573 44.384	54.375	35.202	1.00	58.96
	4698	Ň	ILE D	16	46.006	54.102 55.037	35.367 34.144	1.00	58.96
15	4699	CA	ILE D	16	45.052	55.457	33.146	1.00 1.00	65.25
	4700	СВ	ILE D	16	44.928	56.967	33.117	1.00	65.25
	4701	CG2	ILE D	16	44.319	57.455	34.414	1.00	107.28 107.28
	4702	CG1	ILE D	16	46.303	57.587	32.876	1.00	107.28
00	4703	CD1	ILE D	16	46.295	59.099	32.854	1.00	107.28
20	4704	Ç	ILE D	16	45.380	54.992	31.754	1.00	65.25
	4705	0	ILE D	16	46.492	54.553	31.461	1.00	65.25
	4706.	N	PHE D	17	44.373	55.117	30.905	1.00	82.89
	4707	CA	PHE D	17	44.429	54.750	29.509	1.00	82.89
25	4708	CB CG	PHE D	17	43.011	54.508	29.030	1.00	73.74
23	4709 4710	CD1	PHE D PHE D	17	42.550	53.099	29.186	1.00	73.74
	4711	CD2	PHE D	17 17	41.245	52.822	29.578	1.00	73.74
	4712	CE1	PHE D	17	43.379 40.779	52.052 51.529	28.825	1.00	73.74
	4713	CE2	PHE D	17	42.918	50.741	29.625 28.866	1.00	73.74
30	4714	CZ	PHE D	17	41.609	50.484	29.258	1.00 1.00	73.74
	4715	C	PHE D	17	45.066	55.863	28.677	1.00	73.74 82.89
	4716	0	PHE D	17	45.154	57.009	29.117	1.00	82.89
	4717	N	LYS D	18	45.502	55.531	27.469	1.00	90.77
25	4718	CA	LYS D	18	46.117	56.516	26.588	1.00	90.77
35	4719	CB	LYS D	18	46.681	55.810	25.357	1.00	139.85
	4720	CG	LYS D	18	47.467	56.691	24.410	1.00	139.85
	4721 4722	CD	LYS D	18	48.254	55.822	23.441	1.00	139.85
	4723	CE NZ	LYS D LYS D	18	49.094	56.637	22.472	1.00	139.85
40	4724	C	LYS D	18 18	48.256	57.533 57.550	21.630	1.00	139.85
. •	4725	ŏ	LYS D	18	45.079 43.975	57.556 57.212	26.156	1.00	90.77
	4726	N	GLY D	19	45.420	58.832	25.731 26.284	1.00 1.00	90.77
	4727	CA	GLY D	19	44.501	59.869	25.859	1.00	135.30 135.30
	4728	C	GLY D	19	43.585	60.458	26.909	1.00	135.30
45	4729	0	GLY D	19	42.914	61.451	26.641	1.00	135.30
	4730	N	GLU D	20	43.539	59.863	28.096	1.00	90.73
	4731	CA	GLU D	20	42.679	60.387	29.158	1.00	90.73
	4732	CB	GLU D	20	42.370	59.283	30.165	1.00	145.66
50	4733 4734	CG	GLU D	20	41.858	58.007	29.497	1.00	145.66
50	4735	CD OE1	GLU D	20	41.421	56.945	30.491	1.00	145.66
	4736	OE2	GLU D	20 20	42.233 40.265	56.567	31.363	1.00	145.66
	4737	C	GLU D	20		56.483	30.393	1.00	145.66
	4738	ŏ	GLU D	20	43.339 44.510	61.593 61.887	29.844 29.590	1.00	90.73
55	4739	N	ASN D	21	42.592	62.311	30.682	1.00 1.00	90.73
	4740	CA	ASN D	21	43.163	63.469	31.364	1.00	106.51 106.51
	4741	CB	ASN D	21	42.409	64.761	31.030	1.00	191.80
	4742	CG	ASN D	21	42.014	64.865	29.580	1.00	191.80
60	4743	OD1	ASN D	21	42.781	64.543	28.677	1.00	191.80
60	4744	ND2	ASN D	21	40.797	65.346	29.365	1.00	191.80
	4745	C	ASN D	21	43.127	63.300	32.872	1.00	106.51
	4746 4747	0	ASN D	21	42.165	62.756	33.424	1.00	106.51
	4747 4748	N CA	VAL D	22	44.170	63.792	33.533	1.00	83.07
65	4748 4749	CA CB	VAL D VAL D	22	44.267	63.727	34.984	1.00	83.07
55	4750	CG1	VAL D	22	45.143	62.571	35.425	1.00	85.11
	4751	CG2	VAL D	22 22	46.555 45.134	62.774 82.475	34.923	1.00	85.11
	4752	Č	VAL D	22	45.134 44.885	62.475 65.015	36.937	1.00	85.11
	4753	ŏ	VAL D	22	45.701	65.643	35.514 34.833	1.00 1.00	83.07
70	4754	Ň	THR D	23	44.517	65.401	36.731	1.00	83.07 66.58
							50.751	1.00	66.58

	4755 4756 4757	CA CB OG1	THR D THR D THR D	23 23 23	45.024 43.848 43.036	66.635 67.553 67.717	37.318 37.646	1.00	66.58 160.89
5	4758 4759 4760	CG2 C O	THR D THR D THR D	23 23 23	44.344 45.820 45.330	68.902 66.391 65.718	36.477 38.121 38.598	1.00 1.00 1.00	160.89 160.89 66.58
	4761 4762 4763	N CA CB	LEU D LEU D LEU D	24 24 24	47.035 47.810 49.235	66.923 66.708 66.263	39.498 38.705 39.933	1.00 1.00 1.00	66.58 91.98 91.98
10	4764 4765 4766	CG CD1 CD2	LEU D LEU D	24 24 24	49.491 50.891 48.509	65.315 64.750 64.210	39.632 38.471 38.587 38.476	1.00 1.00 1.00	82.54 82.54 82.54
15	4767 4768 4769	C O N	LEU D LEU D THR D	24 24 25	47.882 48.622 47.131	67.967 68.895 67.992	40.785 40.479 41.873	1.00 1.00 1.00 1.00	82.54 91.98 91.98
	4770 4771 4772	CA CB OG1	THR D THR D THR D	25 25 25	47.122 45.754 44.757	69.153 69.300 69.342	42.732 43.385 42.357	1.00 1.00 1.00	89.48 89.48 145.87 145.87
20	4773 4774 4775	CG2 C O	THR D THR D THR D	25 25 25	45.686 48.199 48.404	70.568 69.028 67.956	44.198 43.794 44.359	1.00 1.00 1.00	145.87 145.87 89.48 89.48
25	4776 4777 4778	N CA C	CYS D CYS D CYS D	26 26 26	48.909 49.942 49.298	70.117 70.082 70.358	44.050 45.070 46.407	1.00 1.00 1.00	125.74 125.74 125.74
23	4779 4780 4781 4782	O CB SG N	CYS D CYS D CYS D	26 26 26	48.415 51.034 52.476	71.196 71.118 70.930	46.512 44.810 45.922	1.00 1.00 1.00	125.74 105.78 105.78
30	4783 4784 4785	CA CB CG	ASN D ASN D ASN D ASN D	27 27 27 27	49.751 49.263 50.450 50.107	69.628 69.743 69.894	47.416 48.776 49.698	1.00 1.00 1.00	184.56 184.56 249.08
	4786 4787 4788	OD1 ND2 C	ASN D ASN D ASN D	27 27 27 27	49.328 50.683 48.283	69.554 68.630 70.281 70.880	51.100 51.334 52.054 49.023	1.00 1.00 1.00	249.08 249.08 249.08
35	4789 4790 4791	O N CA	ASN D GLY D GLY D	27 28 28	48.686 46.995 45.972	71.988 70.600 71.612	49.365 48.844 49.043	1.00 1.00 1.00 1.00	184.56 184.56 249.39
40	4792 4793 4794	C O N	GLY D GLY D ASN D	28 28 29	44.644 44.494 43.674	71.030 70.609 71.006	48.616 47.470 49.524	1.00 1.00 1.00	249.39 249.39 249.39 249.47
	4795 4796 4797	CA CB CG	ASN D ASN D ASN D	29 29 29	42.377 41.619 40.397	70.429 70.112 69.249	49.206 50.497 50.256	1.00 1.00 1.00	249.47 246.79 246.79
45	4798 4799 4800 4801	OD1 ND2 C O	ASN D ASN D ASN D ASN D	29 29 29	40.234 39.536 41.494	68.672 69.146 71.261	49.182 51.262 48.274	1.00 1.00 1.00	246.79 246.79 249.47
50	4802 4803 4804	N CA CB	ASN D ASN D ASN D	29 30 30 30	41.005 41.294 40.437	70.746 72.538 73.386	47.265 48.594 47.766	1.00 1.00 1.00	249.47 206.51 206.51
	4805 4806 4807	CG OD1 ND2	ASN D ASN D ASN D	30 30 30	39.137 38.302 37.878 38.054	73.705 72.469 72.232 71.678	48.518 48.794 49.926 47.757	1.00 1.00 1.00	210.57 210.57 210.57
55	4808 4809 4810	C O N	ASN D ASN D PHE D	30 30 31	41.073 41.381 41.266	74.685 74.848 75.614	47.297 46.115 48.224	1.00 1.00 1.00 1.00	210.57 206.51 206.51 230.41
60	4811 4812 4813	CA CB CG	PHE D	31 31 31	41.829 40.891 39.472	76.899 78.020 77.878	47.860 48.330 47.828	1.00 1.00 1.00	230.41 249.56 249.56
00	4814 4815 4816	CD1 CD2 CE1	PHE D PHE D PHE D	31 31 31	38.588 39.030 37.283	76.991 78.608 76.839	48.440 46.725 47.969	1.00 1.00 1.00	249.56 249.56 249.56
65	4817 4818 4819 4820	CE2 CZ C	PHE D PHE D PHE D PHE D	31 31 31 31	37.727 36.853 43.249	78.463 77.574 77.132	46.245 46.866 48.360	1.00 1.00 1.00	249.56 249.56 230.41
_	4821 4822 4823	N CA CB	PHE D PHE D PHE D	32 32 32	43.542 44.122 45.531 48.392	76.994 77.486 77.753	49.552 47.416 47.683	1.00 1.00 1.00	230.41 186.13 186.13
70	4824	CG	PHE D	32	47.810	76.753 76.726	46.925 47.381	1.00 1.00	237.35 237.35

	4825 4826	CD1 CD2	PHE D	32 32	48.121 48.835	76.283 77.167	48.659 46.552	1.00	237.35
	4827	CE1	PHE D	32	49.434	76.277	49.112	1.00 1.00	237.35
	4828	CE2	PHE D	32	50.156	77.166	46.998	1.00	237.35
5	4829	CZ	PHE D	32	50.454	76.719	48.286	1.00	237.35
	4830	С	PHE D	32	45.909	79.173	47.251	1.00	237.35 186.13
	4831	0	PHE D	32	45.122	79.856	46.601	1.00	186.13
	4832	N	GLU D	33	47.117	79.617	47.595	1.00	249.49
	4833	CA	GLU D	33	47.539	80.969	47.225	1.00	249.49
10	4834	CB	GLU D	33	47.683	81.860	48.457	1.00	249.38
	4835	CG	GLU D	33	47.919	83.321	48.090	1.00	249.38
	4836	CD	GLU D	33	46.730	83.912	47.362	1.00	249.38
	4837 4838	OE1 OE2	GLU D	33	45.593	83.561	47.740	1.00	249.38
15	4839	C	GLU D	33 33	46.914	84.731	46.433	1.00	249.38
15	4840	ŏ	GLU D	33	48.822 48.826	81.120 81.765	46.422	1.00	249.49
	4841	Ň	VAL D	34	49.918	80.566	45.3 7 2 46.929	1.00 1.00	249.49
	4842	CA	VAL D	34	51.194	80.698	46.247	1.00	207.78 207.78
	4843	СВ	VAL D	34	52.284	79.859	46.944	1.00	207.78
20	4844	CG1	VAL D	34	53.608	80.005	46.212	1.00	207.37
	4845	CG2	VAL D	34	52.437	80.316	48.384	1.00	207.37
	4846	C	VAL D	34	51.130	80.333	44.770	1.00	207.78
	4847	0	VAL D	34	50.333	79.492	44.343	1.00	207.78
25	4848	N	SER D	35	51.966	81.007	43.992	1.00	228.15
23	4849	CA	SER D	35	52.043	80.778	42.563	1.00	228.15
	4850 - 4851	CB OG	SER D	35	51.944	82.104	41.810	1.00	249.21
	4852	C	SER D SER D	35 35	53.093	82.901	42.038	1.00	249.21
	4853	ŏ	SER D	35 35	53.386 53.703	80.116	42.275	1.00	228.15
30	4854	Ň	SER D	36	54.1 7 7	79.813 79.906	41.126 43.326	1.00 1.00	228.15
	4855	CA	SER D	36	55.481	79.265	43.185	1.00	238.59 238.59
	4856	СВ	SER D	36	56.552	80.002	43.997	1.00	200.88
	4857	OG	SER D	36	56.368	79.808	45.389	1.00	200.88
~ ~	4858	С	SER D	36	55.395	77.821	43.653	1.00	238.59
35	4859	0	SER D	36	55.568	77.519	44.835	1.00	238.59
	4860	N	THR D	37	55.115	76.935	42.706	1.00	119.38
	4861	CA	THR D	37	55.004	75.514	42.974	1.00	119.38
	4862 4863	CB OG1	THR D	37	53.561	75.034	42.738	1.00	138.47
40	4864	CG2	THR D THR D	37 37	52.664	75.794	43.557	1.00	138.47
10	4865	C	THR D	37	53.426 55.950	73.568	43.078	1.00	138.47
	4866	ŏ	THR D	37	56.054	74.838 75.258	41.992 40.841	1.00 1.00	119.38
	4867	Ň	LYS D	38	56.653	73.808	42,446	1.00	119.38
	4868	CA	LYS D	38	57.594	73.098	41.585	1.00	140,44 140,44
45	4869	CB	LYS D	38	58.938	72.982	42.288	1.00	200.36
	4870	CG	LYS D	38	59.508	74.309	42.714	1.00	200.36
	4871	CD	LYS D	38	60.837	74.125	43.415	1.00	200.36
	4872	CE	LYS D	38	61.449	75.465	43.766	1.00	250.36
50	4873	NZ	LYS D	38	62.770	75.308	44.427	1.00	200.36
50	4874	C	LYS D	38	57.100	71.701	41.218	1.00	140.44
	4875 4878	0 N	LYS D	38	56.507	71.013	42.045	1.00	140.44
	4877		TRP D	39	57.341	71.284	39.976	1.00	125.62
	4878	CA CB	TRP D	39 39	56.934	69.953	39.520	1.00	125.62
55	4879	CG	TRP D	39	55.830 54.540	70.028 70.582	38.470	1.00	111.13
	4880	CD2	TRP D	39	53.645	69.978	38.973 39.915	1.00 1.00	111.13
	4881	CE2	TRP D	39	52.567	70.867	40.090	1.00	111.13
	4882	CE3	TRP D	39	53.651	68.776	40.628	1.00	111.13
	4883	CD1	TRP D	39	53.984	71.774	38.628	1.00	111.13
60	4884	NE1	TRP D	39	52.798	71.953	39.295	1.00	111.13
	4885	CZ2	TRP D	39	51.503	70.588	40.948	1.00	111,13
	4886	CZ3	TRP D	39	52.589	68.503	41.482	1.00	111.13
	4887	CH2	TRP D	39	51.531	69.405	41.633	1.00	111.13
65	4888 4889	C	TRP D	39	58.115	69.240	38.913	1.00	125.62
5 5	4890	N	TRP D PHE D	39	58.809	69.797	38.077	1.00	125.62
	4891	ČA	PHE D	40 40	58.331 59.458	68.000	39.318	1.00	94.48
	4892	CB	PHE D	40	60.475	67.260 66.976	38.800	1.00	94.48
	4893	ČĠ	PHE D	40	60.977	68.203	39.910 40.607	1.00 1.00	162.61
70	4894	CD1	PHE D	40	60.217	68.816	41.594	1.00	162.61 162.61
								1.00	102.01

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	4895	CD2	PHE D	40 -	62.222	68.734	40.292	1.00	162.61
	4896	CE1	PHE D	40	60.687	69.941	42.264	1.00	162.61
	4897	CE2	PHE D	40	62.705	69.859	40.953	1.00	162.61
5	4898	CZ	PHE D	40	61.934	70.465	41.945	1.00	162.61
3	4899	Ç	PHE D	40	59.063	65.951	38,152	1.00	94.48
	4900	0	PHE D	40	59.061	64.906	38.803	1.00	94.48
	4901	N	HIS D	41	58.727	66.006	36.869	1.00	72.94
	4902	CA	HIS D	41	58.368	64.797	36.133	1.00	-72.94
10	4903	CB	HIS D	41	57.649	65.192	34.848	1.00	108.26
10	4904	CG	HIS D	41	57.262	64.034	33.991	1.00	108.26
	4905 4906	CD2 ND1	HIS D	41	57.305	63.866	32.649	1.00	108.26
	4906 4907	CE1	HIS D	41	56.717	62.879	34.507	1.00	108.26
	4908	NE2	HIS D	41 41	56.441	62.049	33.519	1.00	108.26
15	4909	C	HIS D	41	56.788 59.642	62.625	32.381	1.00	108.26
10	4910	ŏ	HIS D	41	60.482	63.973 64.384	35.816	1.00	72.94
	4911	Ň	ASN D	42	59.770	62.805	35.014	1.00	72.94
	4912	CA CA	ASN D	42	60.939	61.934	36.445 36.277	1.00	79.39
	4913	CB	ASN D	42	61.153	61.554	34.808	1.00 1.00	79.39
20	4914	ČĞ	ASN D	42	60.141	60.504	34.327	4.00	100.05
	4915	OD1	ASN D	42	58.962	60.635	34.637	1.00	100.05 100.05
	4916	ND2	ASN D	42	60.578	59.502	33.560	1.00	100.05
	4917	С	ASN D	42	62.190	62.653	36.783	1.00	79.39
	4918	0	ASN D	42	63.298	62.386	36.318	1.00	79.39
25	4919	N	GLY D	43	62.013	63.562	37.739	1.00	194.33
	4920	CA	GLY D	43	63.147	64.294	38.279	1.00	194.33
	4921	С	GLY D	43	63.397	65.624	37.584	1.00	194.33
	4922	0	GLY D	43	63.744	66.616	38.226	1.00	194.33
••	4923	N	SER D	44	63.221	65.644	36.267	1.00	226.19
30	4924	CA	SER D	44	63.422	66.852	35.476	1.00	226.19
	4925	CB	SER D	44	63.315	68.520	33.987	1.00	149.84
	4926	OG.	SER D	44	64.180	65.450	°33.639	1.00	149.84
	4927	Ç	SER D	44	62.376	67.899	35.837	1.00	226.19
35	4928	0	SER D	44	61.179	67.617	35.812	1.00	226.19
22	4929	N	LEU D	45	62.824	69.107	36.172	1.00	151.08
	4930 4931	CA CB	LEV D	45	61.897	70.180	36.531	1.00	151.08
	4932	CG	LEU D	45 45	62.673	71.473	36.830	1.00	168.08
	4933	CD1	LEU D	45 45	61.854 60.980	72.699	37.259	1.00	168.08
40	4934	CD2	LEU D	45	62.788	72.345 73.853	38.451 37.607	1.00 1.00	168.08
	4935	C	LEU D	45	60.885	70.422	35.398	1.00	168.08 151.08
	4936	ŏ	LEU D	45	61.215	70.281	34.219	1.00	151.08
	4937	Ň	SER D	46	59.650	70.772	35.755	1.00	118.65
	4938	CA	SER D	46	58.614	71.032	34.762	1.00	118.65
45	4939	CB	SER D	46	57.279	70.467	35.236	1.00	145.92
	4940	OG	SER D	46	56.288	70.641	34.240	1.00	145.92
	4941	C	SER D	46	58.499	72.537	34.569	1.00	118.65
	4942	0	SER D	46	59.012	73.306	35.378	1.00	118.65
	4943	N	GLU D	47	57.828	72.965	33.505	1.00	181.92
50	4944	CA	GLU D	47	57.679	74.395	33.255	1.00	181.92
	4945	CB	GLU D	47	57.725	74.692	31.746	1.00	232.55
	4946	CG	GLU D	47	58.747	73.882	30.951	1.00	232.55
	4947	CD	GLU D	47	58.494	73.918	29.437	1.00	232.55
55	4948	OE1	GLU D	47	57.657	73.130	28. 94 7	1.00	232.55
22	4949	OE2	GI.U D	47	59.123	74.749	28.747	1.00	232.55
	4950	C	GLU D	47	56.398	74.999	33.858	1.00	181.92
	4951 4952	0 N	GLU D	47	56.185	76.203	33.732	1.00	181.92
	4953	CA	GLU D	48	55.538	74.196	34.492	1.00	100.90
60	4954	CB	GLU D	48 48	54.330 53.184	74.777	35.104	1.00	100.90
00	4955	ČĠ	GLU D	48	51.945	73.753	35.227	1.00	175.62
	4956	CD	GLU D	48	51.173	74.246 75.204	36.025	1.00	175.62
	4957	OE1	GLU D	48	50.544	75.384 75.147	35.355 34.300	1.00	175.62
	4958	OE2	GLU D	48	51.193	76.517	35.887	1.00 1.00	175.62 175.62
65	4959	c c	GLU D	48	54.698	75.309	36.490	1.00	100.90
	4960	ŏ	GLU D	48	55.879	74.868	37.096	1.00	100.90
	4961	N	THR D	49	53.927	76.275	36.977	1.00	145.22
	4962	CA	THR D	49	54.186	76.860	38.287	1.00	145.22
70	4963	СВ	THR D	49	54.710	78.308	38.155	1.00	156.90
70	4964	OG1	THR D	49	53.774	79.094	37.405	1.00	156.90

	4965	CG2	THR D	•••	56.059	78.319	37.442	1.00	156.90
	4966	C	THR D	49	52.921	76.841	39.150	1.00	145.22
	4967	0 .	THR D	49	53.002	76.780	40.384	1.00	145.22
5	4968 4969	N CA	ASN D ASN D	50 50	51.757 50.486	76.881 76.844	38.500 39.213	1.00	138.33
,	4970	CB	ASN D	50	49.323	76.826	38.220	1.00 1.00	138.33
	4971	CG	ASN D	50	47.991	77.129	38.880	1.00	234.43
	4972	OD1	ASN D	50	47.868	77.026	40.100	1.00	234.43 234.43
	4973	ND2	ASN D	50	46.989	77.490	38.081	1.00	234.43
10	4974	C	ASN D	50	50.480	75.564	40.054	1.00	138.33
	4975	Ŏ	ASN D	50	51.104	74.574	39.683	1.00	138.33
	4976	Ñ	SER D	51	49.782	75.578	41.183	1.00	192.24
	4977	CA	SER D	51	49.733	74.400	42.046	1.00	192.24
	4978	СВ	SER D	51	49.042	74.734	43.376	1.00	111.18
15	4979	OG	SER D	51	47.655	74.994	43.211	1.00	111.18
	4980	С	SER D	51	49.023	73.213	41.399	1.00	192.24
	4981	0	SER D	51	49.166	72.078	41.848	1.00	192.24
	4982	N	SER D	52	48.252	73.470	40.351	1.00	99.05
	4983	CA	SER D	52	47.526	72.400	39.677	1.00	99.05
20	4984	CB	SER D	52	46.041	72.765	39.522	1.00	120.15
	4985	OG	SER D	52	45.402	72.880	40.781	1.00	120.15
	4986	C	SER D	52	48.147	72.145	38.314	1.00	99.05
	4987	0	SER D	52	48.052	72.970	37.410	1.00	99.05
25	4988	N	LEU D	53	48.797	70.997	38.183	1.00	107.39
23	4989	CA	LEU D	53	49.443	70.602	36.938	1.00	107.39
	4990	CB	LEU D	53	50.774	69.910	37.246	1.00	80.33
	4991 4992	CG CD1	LEU D	53	51.398	68.972	36.203	1.00	80.33
	4993	CD2	LEU D	53 53	51.298 52.856	69.580	34.817	1.00	80.33
30	4994	C	LEU D	53	48.548	68.675 69.654	36.589 36.158	1.00 1.00	80.33
50	4995	ŏ	LEU D	53	48.472	68,474	36.476	1.00	107.39 107.39
	4996	Ň	ASN D	54	47.876	70.159	35.130	1.00	103.21
	4997	CA	ASN D	54	46.989	69.314	34.339	1.00	103.21
	4998	CB	ASN D	54	45.977	70.162	33.573	1.00	126.61
35	4999	ČĠ	ASN D	54	44.932	70.755	34.475	1.00	126.61
	5000	QD1	ASN D	54	44.260	70.038	35.217	1.00	126.61
	5001	ND2	ASN D	54	44.781	72.072	34.420	1.00	126.61
	5002	C	ASN D	54	47.732	68.434	33.362	1.00	103.21
	5003	0	ASN D	54	48.882	68.690	33.026	1.00	103.21
40	5004	N	ILE D	55	47.056	67.381	32.921	1.00	179.18
	5005	CA	ILE D	55	47.601	66.449	31.947	1.00	179.18
	5006	CB	ILE D	55	48.061	65.127	32.606	1.00	94.31
	5007	CG2	ILE D	5 5	48.187	64.027	31.558	1.00	94.31
45	5008	CG1	ILE D	55	49.393	65.356	33.324	1.00	94.31
45	5009	CD1	ILE D	55	49.946	64.146	34.029	1.00	94 31
	5010	C	ILE D	55	46.473	66.173	30.975	1.00	17 <i>5</i> .18
	5011	0	ILE D	55	45.402	65.719	31.373	1.00	179.18
	5012	N	VAL D	56	46.701	66.476	29.704	1.00	148.36
50	5013 5014	CA	VAL D	56 50	45.674	66.254	28.704	1.00	148.36
50	5014 5015	CB CG1	VAL D VAL D	56	45.589	67.433	27.737	1.00	191.19
	5015 5016	CG2	VAL D	56 56	44.260	67.393 68.734	26.992 28.509	1.00	191.19
	5017	C	VAL D	56	45.729 45.998	64.975	28.509 27. 95 6	1.00 1.00	191.19
	5018	ŏ	VAL D	56	46.797	64.180	28.445	1.00	148.36 148.36
55	3019	Ň	ASN D	57	45.386	64.774	26.789	1.00	142.96
-	5020	CA	ASN D	57	15.604	63.560	25.999	1.00	14z.96
	5021	CB	ASN D	57	45.673	63.895	24.509	1.00	249.24
	5022	ČĞ	ASN D	57	44.331	64.323	23.952	1.00	249.24
	5023	OD1	ASN D	57	43.331	63.617	24.101	1.00	249.24
60	5024	ND2	ASN D	57	44.298	65.482	23.307	1.00	249.24
	5025	С	ASN D	57	46.861	62.815	26,436	1.00	142.96
	5026	Ó	ASN D	57	47.956	63.052	25.919	1.00	142.96
	5027	N	ALA D	58	46.683	61.917	27.403	1.00	155.81
	5028	CA	ALA D	58	47.775	61.140	27.966	1.00	155.81
65	5029	CB	ALA D	58	47.245	60.191	29.002	1.00	45.44
	5030	Ç	ALA D	58	48.595	60.375	26.939	1.00	155.81
	5031	0	ALA D	58	48.086	59.524	26.214	1.00	155.81
	5032	N	LYS D	59	49.881	60.690	26.890	1.00	75.94
70	5033	CA	LYS D	59	50.807	60.036	25.979	1.00	75.94
70	5034	СВ	LYS D	59	51.654	61.085	25.248	1.00	205.66

	5035	CG	LYS D	59	50.830	62,088	24,439	1.00	205.66
	5036	CD	LYS D	59	51.689	63.187	23.829	1.00	205.66
	5037	CE	LYS D	59	50.838	64.174	23.036	1.00	205.66
-	5038	NZ	LYS D	59	51.652	65.278	22.452	1.00	205.66
5	5039	C	LYS D	59	51.673	59.164	26.886	1.00	75.94
	5040	0	LYS D	59	51.945	59.548	28.028	1.00	75.94
	5041	N	PHE D	60	52.082	57.991	26.398	1.00	73.11
	5042	CA	PHE D	60	52.916	57.070	27.183	1.00	73.11
10	5043	CB	PHE D	60	53.521	56.025	26.277	1.00	111.86
10	5044 5045	CG CD1	PHE D	60	52.512	55.131	25.662	1.00	111.86
	5045 5046	CD2	PHE D PHE D	60	52.745	54.540	24.431	1.00	111.86
	5047	CE1	PHE D	60	51.323	54.863	26.314	1.00	111.86
	5048	CE2	PHE D	60 60	51.810 50.379	53.690	23.853	1.00	111.86
15	5049	CZ	PHE D	60	50.622	54.018 53.429	25.750 24.517	1.00	111.86
	5050	Č	PHE D	60	54.026	57.782	27.946	1.00	111.86
	5051	ŏ	PHE D	60	54.401	57.368	29.037	1.00 1.00	73.11
	5052	N	GLU D	61	54.544	58.863	27.369	1.00	73.11 133.04
	5053	CA	GLU D	61	55.611	59.639	27.993	1.00	133.04
20	5054	CB	GLU D	61	56.112	60.736	27.046	1.00	249.40
	5055	CG	GLU D	61	56.707	60.232	25.750	1.00	249.40
	5056	CD	GLU D	61	55.711	59.447	24.926	1.00	249.40
	5057	OE1	GLU D	61·	54.616	59.981	24.643	1.00	249.40
05	5058	OE2	GLU D	61	56.023	58.296	24.561	1.00	249.40
25	5059	Č	GLU D	61	55.162	60.298	29.289	1.00	133.04
	5060	0	GLU D	61	55.995	60.638	30.124	1.00	133.04
	5061	N	ASP D	62	53.854	60.493	29.452	1.00	85.82
	5062	CA	ASP D	62	53.344	61.130	30.659	1.00	85.82
30	5063 5064	CB CG	ASP D	62	51.887	61.546	30.471	1.00	150.56
50	5065	OD1	ASP D ASP D	62 62	51.694	62.436	29.258	1.00	150.56
	5066	OD2	ASP D	62	52.584 50.650	63.274 62.302	28.983	1.00	150.56
	5067	C	ASP D	62	53.484	60.179	28.585 31.838	1.00	150.56
	5068	ŏ	ASP D	62	53.464	60.605	32.999	1.00 1.00	85.82
35	5069	N	SER D	63	53.636	58.888	31.532	1.00	85.82 75.53
	5070	CA	SER D	63	53.798	57.858	32.566	1.00	75.53
	5071	CB	SER D	63	53.958	56.471	31.933	1.00	120.69
	5072	OG	SER D	63	52.776	56.060	31.271	1.00	120.69
40	5073	С	SER D	63	55.064	58.219	33.303	1.00	75.53
40	5074	0	SER D	63	56.071	58.440	32.671	1.00	75.53
	5075	N	GLY D	64	55.038	58.291	34.624	1.00	67.79
	5076	CA	GLY D	64	56.262	58.644	35.318	1.00	67.79
	5077	C	GLY D	64	56.113	58.959	36.798	1.00	67.79
45	5078 5079	0 N	GLY D	64	55.060	58.708	37.391	1.00	67.79
73	5080	CA	GLU D Gごり D	65 65	57.173	59.500	37.396	1.00	63.91
	5081	CB	GLU D	65 65	57.212 58.542	59.843 50.053	38.817	1.00	63.91
	5082	CG	GLU D	65	58.869	59.353 59.830	39.392	1.00	198.27
	5083	CD	GLU D	65	60.319	59.576	40.778 41.129	1.00 1.00	198.27
50	5084	OE1	GLU D	65	61.203	60.162	40.465	1.00	198.27
	5085	OE2	GLU D	65	60.576	58.786	42.061	1.00	198.27 198.27
	5086	Ċ	GLU D	65	57.098	61.355	38.943	1.00	63.91
	5087	0	GLU D	65	57.862	62.078	38.322	1.00	63.91
	5088	N	TYR D	66	56.151	61.849	39.727	1.00	104.89
55	5089	CA	TYR D	66	55.995	63.295	39.869	1.00	104.89
	5090	CB	TYR D	66	54.621	63.739	39.384	1.00	61.05
	5091	CG	TYR D	66	54.348	63.543	37.922	1.00	61.05
	5092	CD1	TYR D	66	54.057	62.291	37.403	1.00	61.05
60	5093	CE1	TYR D	66	53.721	62.142	36.065	1.00	61.05
60	5094	CD2	TYR D	66	54.307	64.633	37.065	1.00	61.05
	5095	CE2	TYR D	66	53.972	64.489	35.737	1.00	61.05
	5096	CZ	TYR D	66	53.679	63.253	35.239	1.00	61.05
	5097 5098	OH C	TYR D TYR D	66	53.338	63.149	33.911	1.00	61.05
65	5099	ŏ	TYR D	66	56.119	63.743	41.314	1.00	104.89
33	5100	Ň	LYS D	66 67	55.990 56.343	62.923 65.046	42.228	1.00	104.89
	5101	CA	LYS D	67 67	56.343 56.437	65.046 65.618	41.518	1.00	107.31
	5102	CB	LYS D	67	57.700	65.618 65.134	42.867 43.562	1.00	107.31
	5103	CG	LYS D	67	58.926	65.307	43.562 42.721	1.00 1.00	121.51
70	5104	CD	LYS D	67	60.124	64.712	43.416	1.00	121.51 121.51
							70.710	1.50	161.51

	5105 5106	CE NZ	LYS D	67 67	61.319 62.482	64.708 64.056	42.491 43.140	1.00	121.51
	5107	Ċ	LYS D	67	56.419	67.137	42.839	1.00 1.00	121.51
-	5108	O	LYS D	67	56.758	67.744	41.836	1.00	107.31 107.31
5	5109	N	CYS D	68	55.994	67.747	43.937	1.00	110.81
	5110	CA	CYS D	68	55.962	69.190	44.011	1.00	110.81
	5111 5112	C	CYS D	68 68	56.694	69.634	45.260	1.00	110.81
	5113	СВ	CYS D	68	56.922 54.518	68.842 69.727	46.170 43.988	1.00 1.00	110.81
10	5114	SG	CYS D	68	53.384	69.216	45.310	1.00	140.31 140.31
	5115	N	GLN D	69	57.093	70.900	45.274	1.00	126.93
	5116	CA	GLN D	69	57.804	71.490	46.396	1.00	126.93
	5117	CB CG	GLN D	69	59.300	71.191	46.281	1.00	112.91
15	5118 5119	CD	GLN D GLN D	69 69	60.185 61.665	72.102	47.115	1.00	112.91
	5120	OE1	GLN D	69	62.131	71.867 71.871	46.875 45.730	1.00 1.00	112.91
	5121	NE2	GLN D	69	62.416	71.667	47.959	1.00	112.91 112.91
	5122	С	GLN D	69	57.566	72.990	46.341	1.00	126.93
20	5123	0	GLN D	69	57.314	73.542	45.269	1.00	126.93
20	5124 5125	N	HIS D	70	57.642	73.652	47.488	1.00	191.71
	5125	CA CB	HIS D	70 70	57.429 56.372	75.090	47.528	1.00	191.71
	.5127	CG	HIS D	70	54.997	75.434 74.961	48.577 48.219	1.00 1.00	178.35
	5128	CD2	HIS D	70	54.315	73.848	48.585	1.00	178.35 178.35
25	5129	ND1	HIS D	70	54.173	75.648	47.353	1.00	178.35
	5130	CE1	HIS D	70	53.041	74.981	47.202	1.00	178.35
	5131 5132	NE2	HIS D	70	53.101	73.886	47.940	1.00	178.35
	5133	C	HIS D	70 70	58.711	75.856 75.000	47.808	1.00	191.71
30	5134	Ň	GLN D	70 71	59.813 58.553	75.299 77.145	47.784 48.068	1.00 1.00	191.71
	5135	CA	GLN D	71	59.681	78.018	48.338	1.00	249.37 249.37
	5136	CB	GLN D	71	59.161	79.419	48.681	1.00	212.46
	5137	CG	GLN D	71	60.101	80.540	48.260	1.00	212.46
35	5138 5139	CD OE1	GLN D	71	60.527	80.432	46.806	1.00	212.46
55	5140	NE2	GLN D GLN D	71 71	59.736 61.786	80.661	45.894	1.00	212.46
	5141	C	GLN D	71	60.570	80.066 77.474	46.587 49.462	1.00 1.00	212.46
	5142	0	GLN D	71	61.775	77.297	49.269	1.00	249.37 249.37
40	5143	N	GLN D	72	59.974	77.195	50.622	1.00	156.64
40	5144	CA	GLN D	72	60.728	76.683	51.771	1.00	156.64
	5145 5146	CB CG	GLN D GLN D	72 72	60.738	77.728	52.895	1.00	249.31
	5147	CD	GLN D	72	61.596 61.612	77.360 78.445	54.104 55.168	1.00	249.31
	5148	OE1	GLN D	72	62.001	79.584	54.904	1.00 1.00	249.31 249.31
45	5149	NE2	GLN D	72	61.187	78.096	56.378	1.00	249.31
	5150	Ç	GLN D	72	60.149	75.374	52.302	1.00	156.64
	5151 5152	0 N	GLN D	72	59.772	75.277	53.472	1.00	156.64
	5152	ČA	VAL D	73	60.084 59.530	74.362	51.446	1.00	234.28
50	5154	CB	VAL D	73	58.026	73.078 73.002	51.852 51.529	1.00 1.00	234.28
	5155	CG1	VAL D	73	57.398	71.832	52.244	1.00	131.77 131.77
	5156	CG2	VAL D	73	57.350	74.292	51.910	1.00	131.77
	5157	C	VAL D	73	60.224	71.930	51.141	1.00	234.28
55	5158 5159	O N	VAL D ASN D	73	60.652	72.060	49.995	1.00	234.28
J J	5160	CA	ASN D	74 74	60.337 60.971	70.802 69.646	51.824	1.00	160.29
	5161	CB	ASN D	74	61.437	68.687	51.228 52.321	1.00 1.00	160.29
	5162	CG	ASN D	74	62.337	69.366	53.332	1.00	140.71 140.71
60	5163	OD1	ASN D	74	63.216	70.152	52.957	1.00	140.71
oo	5164 5165	ND2	ASN D	74	62.130	69.065	54.613	1.00	140.71
	5166	CO	ASN D ASN D	74	59.985	68.964	50.286	1.00	160.29
	5167	Ň	GLU D	74 75	58.839 60.446	68.692 69.711	50.653	1.00	160.29
	5168	CA	GLU D	75 75	59.644	68.711 68.074	49.064 48.028	1.00 1.00	155.73 155.73
65	5169	CB	GLU D	75	60.555	67.631	46.881	1.00	134.99
	5170	CG	GLU D	75	61.940	67.190	47.322	1.00	134.99
	5171	CD	GLU D	75	62.884	66.978	46.149	1.00	134.99
	5172 5173	OE1 OE2	GLU D	75 75	63.056	67.916	45.340	1.00	134.99
70	5174	C C	GLU D	75 75	63.460 58.794	65.875 66.907	46.038	1.00	134.99
		=			30.704		48.520	1.00	155.73

	5175	0	GLU D	75	59.207	66.137	49.385	1.00	155.73
	5176	Ň	SER D	76	57.601	66.792	47.946	1.00	91.19
	5177	CA .	SER D	76	56.635	65.760	48.302	1.00	91.19
_	5178	CB	SER D	76	55.314	66.052	47.619	1.00	86.66
5	5179	OG	SER D	76	55.477	65.917	46.224	1.00	86.66
	5180 5181	C	SER D	76 76	57.050 57.000	64.349	47.909	1.00	91,19
	5182	N	GLU D	76 77	57.892 56.431	64.165 63.362	47.020 48.562	1.00	91.19
	5183	CA	GLU D	77	56.701	61.959	48.272	1.00 1.00	100.72
10	5184	СВ	GLU D	77	55.971	61.046	49.259	1.00	100.72 188.13
	5185	CG	GLU D	77	56.457	61.191	50.694	1.00	188.13
	5186	CD	GLU D	77	57.912	60.781	50.876	1.00	188.13
	5187	OE1	GLU D	<u>77</u>	58.637	60.666	49.867	1.00	188.13
15	5188 5189	OE2 C	GLU D	77 77	58.343	60.589	52.036	1.00	188.13
15	5199	ŏ	GLU D	77 77	56.203 55.012	61.715 61.851	46.857 46.588	1.00	100.72
	5191	Ň	PRO D	78	57.108	61.380	45.928	1.00 1.00	100.72 89.58
	5192	CD	PRO D	78	58.577	61.416	46.096	1.00	142.24
••	5193	CA	PRO D	78	56.752	61.125	44.532	1.00	89.58
20	5194	СВ	PRO D	78	58.018	60.508	43.955	1.00	142.24
	5195	ca	PRO D	78	59.097	61.270	44.669	1.00	142.24
	5196 5197	C O.	PRO D	78 78	55.529 55.169	60.249	44.351	1.00	89.58
	5198	Q. N	VAL D	70 79	54.889	59.471 60.397	45.234 43.201	1.00 1.00	89.58
25	5199	CA	VAL D	79	53.713	59.620	42.893	1.00	92.62 92.62
	5200	CB	VAL D	79	52.466	60.484	42.999	1.00	66.56
	5201	CG1	VAL D	79	51.284	59.785	42.333	1.00	66.56
	5202	CG2	VAL D	79	52.177	60.763	44.458	1.00	66.56
30	5203	C O	VAL D	79	53.834	59.092	41.483	1.00	92.62
30	5204 5205	N	VAL D TYR D	79 80	54.122 53.625	59.880 57.782	40.566 41.295	1.00	92.62
	5206	ĞA	TYR D	80	53.757	57.256	39.952	1.00 1.00	61.19 61.19
	5207	СВ	TYR D	80	54.372	55.878	39.936	1.00	249.26
~ -	5208	CG	TYR D	80	54.869	55.534	38.557	1.00	249.26
35	5209	CD1	TYR D	80	55.895	56.275	37.979	1.00	249.26
	5210	CE1	TYR D	80	56.370	55.971	36.708	1.00	249.26
	5211 5212	CD2 CE2	TYR D TYR D	80 80	54.335 54.829	54.491 54.208	37.816 36.532	1.00	249.26
	5213	CZ	TYR D	80	55.822	54.920	35.993	1.00 1.00	249.26 249.26
40	5214	OH	TYR D	80	56.359	54.647	34.755	1.00	249.26
	5215	С	TYR D	80	52.471	57.184	39.194	1.00	61.19
	5216	0	TYR D	80	51.448	56.804	39.737	1.00	61.19
	5217	N	LEU D	81	52.529	57.540	37.924	1.00	59.82
45	5218 5219	CA CB	LEU D	81	51.354	57.492	37.090	1.00	59.82
73	5220	CG	LEU D	81 81	51.089 49.972	58. 875 58.868	36.535 35.515	1.00 1.00	66.30 68.30
	5221	CD1	LEU D	81	48,705	58.435	36.202	1.00	68.30
	5222	CD2	LEU D	81	49.808	60.240	34.932	1.00	66.30
50	5223	Ç	LEU D	81	51.664	56.531	35.945	1.00	59.82
50	5224	0	LEU D	81	52.715	56.663	35.333	1.00	59.82
	5225 5226	· N	GLU D	82	50.795	55.561	35.658	1.00	81.20
	5227	CA CB	GLU D	82 82	51.069 51.229	54.640 53.211	34.557	1.00	81.20
	5228	CG	GLU D	82	52.081	52.353	35.072 34.149	1.00 1.00	125.93 125.93
55	5229	CD	GLU D	82	52.264	50.938	34.661	1.00	125.93
	5230	OE1	GLU D	82	52.389	50.771	35.897	1.00	125.93
	5231	OE2	GLU D	82	52.299	50.001	33.829	1.00	125.93
	5232	C	GLU D	82	49.959	54.695	33.498	1.00	81.20
60	5233 5234	O N	GLU D VAL D	82	48.765	54.633	33.821	1.00	81.20
QO.	5235	CA	VAL D	83 83	50.348 49.379	54.809 54.891	32.230 31.140	1.00 1.00	74.09 74.09
	5236	CB	VAL D	83	49.747	56.013	30.177	1.00	86.03
	5237	CG1	VAL D	83	48.810	55.997	28.998	1.00	86.03
4	5238	CG2	VAL D	83	49.675	57.340	30.895	1.00	86.03
65	5239	C	VAL D	83	49.250	53.603	30.340	1.00	74.09
	5240 5241	O	VAL D	83	50.237	53.000	29.949	1.00	74.09
	5241 5242	N CA	PHE D	84 84	48.023 47.811	53.191 51.957	30.067 29.331	1.00	81.44
	5243	CB	PHE D	84	47.087	51.957 50.944	29.331 30.191	1.00 1.00	81.44 68.59
70	5244	ČĞ	PHE D	84	47.803	50.598	31.437	1.00	68.59
									JJ.55

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	5245	CD1	PHE D	84	47.835	51.485	32,486	1.00	68.59
	5246	CD2	PHE D	84	48.418	49.359	31.583	1.00	68.59
	5247	CE1	PHE D	84	48.470	51.153	33.667	1.00	68.59
5	5248	CE2	PHE D	84	49.058	49.016	32.765	1.00	68.59
,	5249 5250	CZ C	PHE D PHE D	84	49.078	49.917	33.809	1.00	68.59
	5251	ŏ	PHE D	84 84	47.029 46.324	52.029 52.998	28.041	1.00	81.44
	5252	Ň	SER D	85	47.149	52.996	27.746 27.301	1.00 1.00	81.44
	5253	CA	SER D	85	46.462	50.731	26.049	1.00	99.54
10	5254	СВ	SER D	85	47.414	50.901	24.866	1.00	99.54 104.48
	5255	OG	SER D	85	46.741	50.652	23.644	1.00	104.48
	5256	C	SER D	85	46.015	49.277	26.155	1.00	99.54
	5257	0	SER D	85	46.843	48.362	26.130	1.00	99.54
15	5258	N	ASP D	86	44.713	49.067	26.315	1.00	64.12
13	5259 5260	CA CB	ASP D ASP D	86	44.166	47.724	26.426	1.00	64.12
	5260 5261	CG	ASP D ASP D	86 86	44.715 44.939	47.030 45.556	27.676	1.00	91.49
	5262	OD1	ASP D	86	43.981	45.556 44.874	27.454 27.027	1.00	91.49
	5263	OD2	ASP D	86	46.065	·- 077	27.697	1.00 1.00	91.49
20	5264	C	ASP D	86	42.631	47.816	26.481	1.00	91.49 64.12
	5265	0	ASP D	86	42.085	48.907	26.673	1.00	64.12
	5266	N	TRP D	87	41.937	46.686	26.293	1.00	76.92
	5267	CA	TRP D	87	40.470	46.689	26.321	1.00	76.92
25	5268	CB	TRP D	87	39.893	45.330	25.950	1.00	235.26
25	5269 5270	CD2	TRP D	87	39.745	45.196	24.519	1.00	235.26
	5270 5271	CE2	TRP D TRP D	87 87	40.716	44.672	23.629	1.00	235.26
	5272	CE3	TRP D	87	40.219 41.945	44.865 44.025	22.334	1.00	235.26
	5273	CD1	TRP D	87	38.730	45.693	23.805 23.748	1.00 1.00	235.26
30	5274	NE1	TRP D	87	39.014	45.491	22.409	1.00	235.26 235.26
	5275	CZ2	TRP D	87	40.942	44.480	21,244	1.00	235,26
	5276	CZ3	TRP D	87	42.651	43.619	22.683	1.00	235.26
	5277	CH2	TRP D	87	42.147	43.865	21,422	1.00	235.26
35	5278	C	TRP D	87	39.956	47.074	27.680	1.00	76.92
55	5279 5280	0 N	TRP D LEU D	87	39.124	47.968	27.818	1.00	76.92
	5281	CA	LEU D	88 88	40.465 40.070	46.386	28.690	1.00	86.84
	5282	CB	LEU D	88	39.344	46.643 45.435	30.064 30.635	1.00 1.00	86.84
	5283	ČĞ	LEU D	88	38.028	45.109	29.953	1.00	73.66
40	5284	CD1	LEU D	88	37.368	43.952	30.664	1.00	73.66 73.66
	5285	CD2	LEU D	88	37.156	46.335	29.991	1.00	73.66
	5286	Ç	LEU D	88	41.248	46.962	30.953	1.00	86.84
	5287	0	LEU D	88	42.330	46.396	30.820	1.00	86.84
45	5288 5289	N	LEU D	89	41.022	47.870	31.883	1.00	45.19
73	5290	CA CB	LEU D	89	42.067	48.266	32.809	1.00	45.19
	5291	CG	LEU D	89 89	42.573 43.628	49.655 50.105	32.473	1.00	158.38
	5292	CD1	LEU D	89	44.671	49.002	33.471 33.642	1.00	158.38
	5293	CD2	LEU D	89	44.255	51.392	32.982	1.00 1.00	158.38
50	5294	C	LEU D	89	41.502	48.263	34.219	1.00	158.38 45.19
	5295	0	LEU D	89	40.455	48.848	34.463	1.00	45.19
	5296	N	LEU D	90	42.164	47.592	35.153	1.00	80.53
	5297	CA	LEU D	90	41.666	47.579	36.523	1.00	80.53
55	5298 5299	CB	LEU D	90	42.086	46.305	37.234	1.00	38.85
55	5300	CG CD1	LEU D	90	41.710	46.256	38.724	1.00	38.85
	5301	CD2	LEU D	90 90	40.189 42.228	46.295 45.003	38.793	1.00	38.85
	5302	C	LEU D	90	42.245	45.002 48.766	39.432 37.280	1.00	38.85
	5303	Ŏ	LEU D	90	43.445	48.858	37.467	1.00 1.00	80.53 80.53
60	5304	N	GLN D	91	41.400	49.670	37.742	1.00	44.32
	5305	CA	GLN D	91	41.899	50.833	38.464	1.00	44.32
	5306	CB	GLN D	91	41.209	52.089	37.953	1.00	57.44
	5307	CG	GLN D	91	41.391	52.283	36.487	1.00	57.44
65	5308 5309	CD	GLN D	91	40.897	53.611	36.016	1.00	57.44
05	5310	OE1 NE2	GLN D GLN D	91	39.700	53.857	35.979	1.00	57.44
	5311	C	GLN D	91 91	41.816 41.895	54.489	35.664	1.00	57.44
	5312	ŏ	GLN D	91	41.685 40.691	50.714 50.176	39.963 40.435	1.00	44.32
	5313	Ň	ALA D	92	42.613	50.176 51.230	40.435 40.737	1.00	44.32
70	5314	CA	ALA D	92	42.451	51.152	40.737 42.169	1.00 1.00	48.50 48.50
									70.00

	5315	СВ	ALA D	92	43,463	50.199	42.739	1.00	52.70
	5316	C	ALA D	92	42.636	52.538	42.787	1.00	48.50
	5317	0	ALA D	92	43.475	53.347	42.341	1.00	48.50
5	5318	N .	SER D	93	41.846	52.825	43.811	1.00	53.99
2	5319	CA	SER D	93	41.960	54.102	44.481	1.00	53.99
	5320 5321	CB OG	SER D	93	41.048	54.158 53.030	45.713	1.00	83.49
	5322	C	SER D	93 93	41.207 43.412	53.030 54.212	46.543	1.00	83.49
	5323	ŏ	SER D	93	44.134	55.046	44.877 44.361	1.00 1.00	53.99
10	5324	Ň	ALA D	94	43.850	53.338	45.764	1.00	53.99 62.76
	5325	CA	ALA D	94	45.232	53.342	46.220	1.00	62.76
	5326	СВ	ALA D	94	45.301	53.851	47.636	1.00	112.27
	5327	C	ALA D	94	45.723	51.909	46.150	1.00	62.76
15	5328	0	ALA D	94	44.942	50.990	46.361	1.00	62.76
13	5329 5330	N CA	GLU D	95 05	47.006	51.704	45.854	1.00	73.31
	5331	CB	GLU D	95 95	47.535 48.677	50.339 50.301	45.746 44.746	1.00	73.31
	5332	CG	GLU D	95	48.262	50.756	43.364	1.00 1.00	116.96
	5333	CL	GLU D	95	49.287	50.405	42.301	1.00	116.96 116.96
20	5334	OE1	GLU D	95	49.057	50.758	41.121	1.00	116.96
	5335	OE2	GLU D	95	50.320	49.776	42,643	1.00	116.96
	5336	C	GLU D	95	47.987	49.724	47.063	1.00	73.31
	5337	0	GLU D	95	48.194	48.517	47.143	1.00	73.31
25	5338 5339	N CA	VAL D	96 06	48.139 48.557	50.563	48.089	1.00	71.30
23	5340	CB	VAL D	96 96	50.010	50.126 50.433	49.422 49.657	1.00	71.30
	5341	CG1	VAL D	96	50.502	49.611	50.812	1.00 1.00	83.19 83.19
	5342	CG2	VAL D	96	50.802	50.132	48.410	1.00	83.19
	5343	С	VAL D	96	47.713	50.869	50.435	1.00	71.30
30	5344	0	VAL D	96	47.560	52.071	50.347	1.00	71.30
	5345	N	VAL D	97	47.190	50.159	51.420	1.00	69.41
	5346 5347	CA	VAL D	97	46.277	50.778	52.365	1.00	69.41
	5347 5348	CB CG1	VAL D	97 97	44.849 43.889	50.417	51.970	1.00	60.29
35	5349	CG2	VAL D	97	44.654	51.256 50.562	52.717 50.501	1.00 1.00	60.29
	5350	č	VAL D	97	46.410	50.374	53.828	1.00	60.29 69.41
	5351	0	VAL D	97	46.540	49.185	54.136	1.00	69.41
	5352	N	MET D	98	46.316	51.350	54.730	1.00	72.66
40	5353	CA	MET D	98	46.389	51.084	56.169	1.00	72.66
40	5354 5355	CB CC	MET D	98	46.498	52.404	56.921	1.00	249.19
	5355 5356	CG SD	MET D	98	47.751	53.177	56.594	1.00	249.19
	5357	CE	MET D	98 98	49.140 48.761	¹ 52.518 53.180	57.501 50.133	1.00	249.19
	5358	č	MET D	98	45.110	50.363	59.122 56.592	1.00 1.00	249.19 72.66
45	5359	Ö	MET D	98	44.014	50.780	56.201	1.00	72.66 72.66
	5360	N	GLU D	99	45.234	49.288	57.373	1.00	68.49
	5361	CA	GLU D	99	44.063	48.535	57.828	1.00	68.49
	5362	CB	GLU D	99	44.441	47.605	58.977	1.00	249.24
50	5363 5364	CG CD	GLU D	99	43.474	46.454	59.176	1.00	249.24
50	5365	OE1	GLU D	99 99	43.683 44.852	45.744	60.499	1.00	249.24
	5366	OE2	GLU D	99	42.679	45.590 45.331	60.913 61.120	1.00	249.24
	5367	. c	GLU D	99	43.007	49.529	58.315	1.00 1.00	24 9.2 4 68.49
	5368	0	GLU D	99	43.308	50.396	59.129	1.00	68.49
55	5369	N	GLY D	100	41.786	49.439	57.807	1.00	99.19
	5370	CA	GLY D	100	40.757	50.360	58.251	1.00	99.19
	5371	C	GLY D	100	40.336	51.428	57.256	1.00	99.19
	5372 5373	0 0	GLY D	100	39.252	52.016	57.398	1.00	99.19
60	5374	CA	GLN D	101 101	41.167 40.845	51.678 52.709	56.244	1.00	64.03
	5375	CB	GLN D	101	42.121	53.294	55.249 54.653	1.00 1.00	64.03 115.74
	5376	CG	GLN D	101	42.956	54.053	55.650	1.00	115.74
	5377	CD	GLN D	101	42.145	55.055	56.435	1.00	115.74
	5378	OE1	GLN D	101	41.427	54.698	57.365	1.00	115.74
65	5379	NE2	GLN D	101	42.246	56.318	56.053	1.00	115.74
	5380	C	GLN D	101	39.939	52.240	54.118	1.00	64.03
	5381 5382	O N	GLN D PRO D	101	39.701	51.050	53.960	1.00	64.03
	5383	CD	PRO D	102 102	39.411 39.527	53.178 54.647	53.317	1.00	85.32
70	5384	CA	PRO D	102	38.536	54.047 52.761	53.374 52.218	1.00 1.00	90.00 85.32
						J	JE.E 10	1.00	03.32

	5385	CB	PRO D	102	37.759	54.032	51.911	1.00	90.00
	5386 5387	ça	PRO D	102	38.814	55.078	52.098	1.00	90.00
	5388	C .	PRO D	102	39.365	52.273	51.026	1.00	85.32
5	5389	Ň	LEU D	102 103	40.528	52.659	50.867	1.00	85.32
,	5390	CA	LEU D	103	38.760 39.424	51.430 50.003	50.194	1.00	84.38
	5391	CB	LEU D	103	39.973	50.903 49.525	49.016	1.00	84.38
	5392	CG	LEU D	103	40.655	48.977	49.315 48.070	1.00	75.67
	5393	CD1	LEU D	103	41.849	49.845	47.739	1.00	75.67
10	5394	CD2	LEU D	103	41.095	47.543	48.305	1.00 1.00	75.67
	5395	C	LEU D	103	38.467	50.792	47.854	1.00	75.67
	5396	0	LEU D	103	37.453	50.135	47.974	1.00	84.38
	5397	N	PHE D	104	38.771	51.419	46.728	1.00	84.38
	5398	CA	PHE D	104	37.865	51.312	45.586	1.00	75.73 75.73
15	5399	CB	PHE D	104	37.272	52.679	45.208	1.00	163.52
	5400	CG	PHE D	104	36.530	53.359	46.322	1.00	163.52
	5401	CD1	PHE D	104	37.222	53.984	47.352	1.00	163.52
	5402	CD2	PHE D	104	35.139	53.381	46.342	1.00	163.52
20	5403	CE1	PHE D	104	36.542	54.625	48.393	1.00	163.52
20	5404	CE2	PHE D	104	34.446	54.020	47.381	1.00	163.52
	5405	cz	PHE D	104	35.152	54.643	48.407	1.00	163.52
	5406 5407	CO	PHE D	104	38.550	50.717	44.353	1.00	75.73
	5407	Ň	PHE D	104	39.617	51.181	43.942	1.00	75.73
25	5409	CA	LEU D	105	37.950	49.684	43.769	1.00	46.40
	5410	CB	LEU D	105 105	38.504	49.069	42.561	1.00	46.40
	5411	CG	LEU D	105	38. 633 39.461	47.555 47.169	42.722	1.00	51.89
	5412	CD1	LEU D	105	39.723	47.169 45.660	43.932	1.00	51.89
	5413	CD2	LEU D	105	40.750	47.942	43.969 43.836	1.00	51.89
30	5414	C	LEU D	105	37.518	49.366	41.456	1.00 1.00	51.89
	5415	0	LEU D	105	36.330	49.413	41.701	1.00	46.40
	5416	N	ARG D	106	37.988	49.551	40.236	1.00	46.40 68.20
	5417	CA	ARG D	106	37.073	49.852	39.159	1.00	68.20
0.5	5418	CB	ARG D	106	37.090	51.354	38.922	1.00	103.77
35	5419	CG	ARG D	106	36.259	51.801	37.762	1.00	103.77
	5420	CD	ARG D	106	36.514	53.271	37.452	1.00	103.77
	5421	NE	ARG D	106	35.766	53.701	36.275	1.00	103.77
	5422	CZ	ARG D	106	36.095	54.738	35.519	1.00	103.77
40	5423	NH1	ARG D	106	37.170	55.458	35.811	1.00	103.77
+0	5424 5425	NH2	ARG D	106	35.353	55.044	34.462	1.00	103.77
	5425 5426	C	ARG D	106	37.457	49.119	37.876	1.00	68.20
	5427	Ň	ARG D CYS D	106	38.595	49.240	37.415	1.00	68.20
	5428	CA	CYS D	107 107	36.535 36.842	48.340	37.309	1.00	54.86
45	5429	Č	CYS D	107	36.528	47.659 48.688	36.053	1.00	54.86
	5430	ŏ	CYS D	107	35.365	49.000	34.983	1.00	54.86
	5431	CB	CYS D	107	35.984	46.421	34.720 35.850	1.00	54.86
	5432	SG	CYS D	107	36.664	45.289	34.601	1.00 1.00	81.59
	5433	N	HIS D	108	37.578	49.236	34.384	1.00	81.59
50	5434	CA	HIS D	108	37,449	50.285	33.386	1.00	77.64 77.64
	5435	CB	HIS D	108	38.460	51.352	33.687	1.00	84.93
	5436	CG	HIS D	108	38.301	52.573	32.853	1.00	84.93
	5437	CD2	HIS D	108	39.176	53.230	32.060	1.00	84.93
55	5438	ND1	HIS D	108	37.136	53.301	32.834	1.00	84.93
55	5439	CE1	HIS D	108	37.306	54.364	32.068	1.00	84.93
	5440	NE2	HIS D	108	38.534	54.346	31.587	1.00	84.93
	5441	C	HIS D	108	37.608	49.848	31.945	1.00	77.64
	5442 5443	0	HIS D	108	38.604	49.229	31.559	1.00	77.64
60	5444	N CA	GLY D	109	36.618	50.206	31.143	1.00	64.08
00	5445	CA	GLY D	109	36.637	49.820	29.750	1.00	64.08
	5446	C O	GLY D	109	37.367	50.854	28.945	1.00	64.08
	5447	N	TRP D	109	37.498	52.002	29.379	1.00	64.08
	5448	GA CA	TRP D	110 110	37.858 38.575	50.446	27.781	1.00	110.56
65	5449	CB	TRP D	110	39.206	51.353 50.579	26.906	1.00	110.56
	5450	ČĞ	TRP D	110	39.819	50.578 51.458	25.749	1.00	129.78
	5451	CD2	TRP D	110	41.184	51.456 51.879	24.721	1.00	129.78
	5452	CE2	TRP D	110	41.307	52.743	24.659 23.557	1.00	129.78
~ c	5453	CE3	TRP D	110	42.322	51.608	25.557 25.434	1.00 1.00	129.78
70	5454	CD1	TRP D	110	39.184	52.062	23.682	1.00	129.78
							20.002	1.00	129.78

	5455	NE1	TRP D	110 -	40.068	52.836	22.977	1.00	129.78
	5456	CZ2	TRP D	110	42.514	53.345	23.204	1.00	129.78
	5457	CZ3	TRP D	110	43.525	52.208	25.083	1.00	129.78
5	5458 5459	CH2 ·	TRP D	110	43.609	53.068	23.980	1.00	129.78
,	5460	ŏ	TRP D	110 110	37.623 36.417	52.414 52.183	26.377 26.252	1.00	110.56
	5461	Ň	ARG D	111	38.170	53.591	26.232	1.00 1.00	110.56
	5462	CA	ARG D	111	37.377	54.696	25.564	1.00	110.12 110.12
10	5463	CB	ARG D	111	37.068	54.455	24.113	1.00	249.23
10	5464 5465	CG CD	ARG D	111	38.127	54.981	23.233	1.00	249.23
	5466	NE NE	ARG D ARG D	111 111	37.639 38.039	54.963 56.180	21.844	1.00	249.23
	5467	CZ	ARG D	111	37.564	57.390	21.160 21.444	1.00 1.00	249.23
	5468	NH1	ARG D	111	36.661	57.561	22.411	1.00	249.23 249.23
15	5469	NH2	ARG D	111	38.007	58.437	20.760	1.00	249.23
	5470	C	ARG D	111	36.070	54.939	26.286	1.00	110.12
	5471 5472	0 N	ARG D ASN D	111	35.117	55.496	25.736	1.00	110.12
	5473	CA	ASN D	112 112	36.031 34.859	54.502 54.663	27.527 28.349	1.00	80.55
20	5474	CB	ASN D	112	34.546	56.137	28.546	1.00 1.00	80.55 68.20
	5475	CG	ASN D	112	33.765	56.379	29.815	1.00	69.20
	5476	OD1	ASN D	112	33.075	55.484	30.307	1.00	69.20
	5477	ND2	ASN D	112	33.863	57.586	30.355	1.00	69.20
25	5478 5479	C 0	ASN D . ASN D		33.621	53.963	27.813	1.00	80.55
23	5480	N	TRP D	112 113	32.500 33.5⊶	54.357 52.930	28,143	1.00	80.55
	5481	CA	TRP D	113	32.649	52.207	26.998 26.504	1.00 1.00	104.63
	5482	CB	TRP D	113	33.045	51.128	25.519	1.00	104.63 141.29
20	5483	CG	TRP D	113	33.355	51.652	24.198	1.00	141.29
30	5484	CD2	TRP D	113	34.368	51.180	23.311	1.00	141.29
	5485 5486	CE2 CE3	TRP D	113	34.278	51.944	22.133	1.00	141.29
	5487	CD1	TRP D	113 113	35.343 32.705	50.182 52.655	23.397	1.00	141.29
	5488	NE1	TRP D	113	33.254	52.837	23.541 22.296	1.00 1.00	141.29
35	5489	CZ2	TRP D	113	35.126	51.743	21.057	1.00	141.29 141.29
	5490	CZ3	TRP D	113	36.188	49.984	22.324	1.00	141.29
	5491	CH2	TRP D	113	36.075	50.761	21.173	1.00	141.29
	5492 5493	C	TRP D	113	31.928	51.542	27.656	1.00	104.63
40	5494	Ň	ASP D	113 114	32.215 30.990	51.80 6 50.668	28.828 27.313	1.00	104.63
	5495	CA	ASP D	114	30.229	49.960	28.320	1.00 1.00	117.64 117.64
	5496	CB	ASP D	114	28.725	50.109	28.065	1.00	192.42
	5497	CG	ASP D	114	28.176	51.431	28.576	1.00	192.42
45	5498	OD1	ASP D	114	28.288	51.685	29.796	1.00	192.42
40	5499 5500	OD2 C	ASP D	114 114	27.636	52.214	27.764	1.00	192.42
	5501	ŏ	ASP D	114	30.619 30.831	48.498 47.875	28.345 27.301	1.00 1.00	117.64
	5502	Ň	VAL D	115	30.730	47.967	29.559	1.00	117.64 73.71
	5503	CA	VAL D	115	31.084	46.577	29.766	1.00	73.71
50	5504	CB	VAL D	115	32.340	46.448	30.614	1.00	75.80
	5505 5506	CG1	VAL D	115	32.827	45.011	30.593	1.00	75.80
	5507	CG2 C	VAL D VAL D	115	33.403	47.378 45.863	30.086	1.00	75.80
	5508	ŏ	VAL D	115 115	29.947 29.301	45.862 46.431	30.481 31.368	1.00	73,71
55	5509	Ň	TYR D	116	29.700	44.615	30.078	1.00 1.00	73.71 69.51
	5510	CA	TYR D	116	28.642	43.810	30.672	1.00	69.51
	5511	CB	TYR D	116	27.563	43.539	29.638	1.00	100.20
	5512	CG	TYR D	116	26.886	44.780	29.133	1.00	100.20
60	5513 5514	CD1 CE1	TYR D TYR D	116 116	27.276	45.376 48.540	27.942	1.00	100.20
00	5515	CD2	TYR D	116	28.660 25.866	46.549 45.375	27.481 29.858	1.00	100.20
	5516	CE2	TYR D	116	25.243	46.545	29.412	1.00 1.00	100.20 100.20
	5517	CZ	TYR D	116	25.648	47.127	28.225	1.00	100.20
45	5518	ОН	TYR D	116	25.060	48.293	27.795	1.00	100.20
65	5519 5520	C	TYR D	116	29.179	42.488	31.222	1.00	69.51
	5520 5521	0 N	TYR D LYS D	116	30.341	42.127	30.986	1.00	69.51
	5522	CA	LYS D	117 117	28.327 28.708	41.766 40.492	31.947	1.00	88.92
Δ	5523	CB	LYS D	117	28.772	40.492 39.397	32,541 31,480	1.00 1.00	88.92 111.93
70	5524	CG	LYS D	117	27.453	38.715	31.180	1.00	111.93
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	5525	CD	LYS D	117	27.695	37.387	30.471	4.00	444.00
	5526	CE	LYS D	117	28.540	36.435	31.338	1.00 1.00	111.93 111.93
	5527	NZ	LYS D	117	28.852	35.125	30.675	1.00	111.93
_	5528	C .	LYS D	117	30.069	40.625	33.213	1.00	88.92
5	5529	0	LYS D	117	31.002	39.882	32.909	1.00	88.92
	5530	N	VAL D	118	30.182	41.578	34.129	1.00	81.88
	5531	CA	VAL D	118	31.433	41.816	34.828	1.00	81.88
	5532	CB	VAL D	118	31.524	43.274	35.241	1.00	84.78
10	5533	CG1	VAL D	118	32.404	43.434	36.459	1.00	84.78
10	5534	CG2	VAL D	118	32.104	44.055	34.101	1.00	84.78
	5535 5536	C	VAL D	118	31.693	40.949	36.052	1.00	81.88
	5537	Ň	VAL D	118	30.803	40.742	36.893	1.00	81.88
	5538	CA	ILE D	119	32.928	40.468	36.171	1.00	56.52
15	5539	CB	ILE D	119 119	33.296 33.364	39.637 38.181	37.310	1.00	56.52
	5540	CG2	ILE D	119	33.652	37.309	36.895	1.00	59.73
	5541	CG1	ILE D	119	32.058	37.776	38.094	1.00	59.73
	5542	CD1	ILE D	119	32.154	36.446	36.217 35.534	1.00 1.00	59.73
	5543	C	ILE D	119	34.662	40.027	37.826	1.00	59.73
20	5544	0	ILE D	119	35.611	40.026	37.057	1.00	56.52
	5545	N	TYR D	120	34.785	40.378	39.104	1.00	56.52
	5546	CA	TYR D	120	36.115	40.736	39.618	1.00	51.66 51.66
	5547	CB	TYR D	120	36.064	41.770	40.742	1.00	57.63
	5548	CG	TYR D	120	35.658	43.139	40.320	1.00	57.63
25	5549	CD1	TYR D	120	34.336	43.470	40.170	1.00	57.63
	5550	CE1	TYR D	120	33.960	44.720	39.744	1.00	57.63
	5551	CD2	TYR D	120	36.599	44.093	40.038	1.00	57.63
	5552	CE2	TYR D	120	36.237	45.353	39.609	1.00	57.63
20	5553	CZ	TYR D	120	34.915	45.656	39.464	1.00	57.63
30	5554	ОH	TYR D	120	34.549	46.902	39.039	1.00	57.63
	5555	Ç	TYR D	120	36.702	39.486	40.200	1.00	51.66
	5556	0	TYR D	120	35.971	38.657	40.725	1.00	51.66
	5557 5558	N	TYR D	121	38.015	39.353	40.123	1.00	46.59
35	5559	CA CB	TYR D	121	38.667	38.180	40.684	1.00	46.59
55	5560	CG	TYR D	121	39.304	37.344	39.572	1.00	81.03
	5561	CD1	TYR D TYR D	121 121	38.357	36.640	38.623	1.00	81.03
	5562	CE1	TYR D	121	37.541 36.705	37.362 36.721	37.761	1.00	81.03
	5563	CD2	TYR D	121	38.311	35.244	36.856 38.562	1.00 1.00	81.03
40	5564	CE2	TYR D	121	37.478	34.597	37.666	1.00	81.03
	5565	CZ	TYR D	121	36.672	35.345	36.808	1.00	81.03
	5566	OH	TYR D	121	35.835	34.720	35.894	1.00	81.03 81.03
	5567	С	TYR D	121	39.771	38.566	41.683	1.00	46.59
	5568	0	TYR D	121	40.518	39.538	41.473	1.00	46.59
45	5569	N	LYS D	122	39.876	37.809	42.770	1.00	72.20
	5570	CA	LYS D	122	40.920	38.054	43.759	1.00	72.20
	5571	CB	LYS D	122	40.357	38.585	45.073	1.00	128.16
	5572	CG	LYS D	122	41.440	38.842	46.100	1.00	128.16
50	5573	CD	LYS D	122	40.869	39.066	47.470	1.00	128.16
50	5574 5575	CE	LYS D	122	41.973	39.176	48.496	1.00	128.16
	5575 5576	NZ C	LYS D LYS D	122	41.394	39.233	49.865	1.00	128.16
	5577	ŏ	LYS D LYS D	122	41.598	36.736	44.028	1.00	72.20
	5578	Ň	ASP D	122 123	40.977	35.813	44.536	1.00	72.20
55	5579	ČA	ASP D	123	42.876	36.658 35.450	43.692	1.00	101.46
	5580	CB	ASP D	123	43.660 43.802	35.450 35.135	43.884	1.00	101.46
	5581	CG	ASP D	123	44.795	35.135 36.049	45.375	1.00	177.22
	5582	OD1	ASP D	123	45.903	36.238	46.065 45.518	1.00	177.22
	5583	OD2	ASP D	123	44.477	36.572	47.154	1.00 1.00	177.22
60	5584	C	ASP D	123	43.079	34.258	43.138	1.00	177.22 101.46
	5585	0	ASP D	123	43.017	33.147	43.668	1.00	101.46
	5586	N	GLY D	124	42.661	34.502	41.898	1.00	89.52
	5587	CA	GLY D	124	42.103	33.456	41.056	1.00	89.52
	5588	С	GLY D	124	40.673	33.041	41.346	1.00	89.52
65	5589	0	GLY D	124	40.092	32.261	40.587	1.00	89.52
	5590	N	GLU D	125	40.097	33.559	42.428	1.00	72.85
	5591	CA	GLU D	125	38.730	33.206	42.826	1.00	72.85
	5592	CB	GLU D	125	38.599	33.194	44.362	1.00	232.74
70	5593	CG	GLU D	125	39.348	32.082	45.103	1.00	232.74
70	5594	CD	GLU D	125	38.625	30.746	45.068	1.00	232.74
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	5595	OE1	GLU D	105	27 402	20.000	40.000		
	5596	OE2	GLU D	125 125	37.493 39.194	30.662	45.593	1.00	232.74
	5597	č	GLU D	125	37.706	29.780 34.202	44.517 42.280	1.00	232.74
	5598	ŏ.	GLU D	125	37.974	35.404	42.280	1.00	72.85
5	5599	N	ALA D	126	36.527	33.708	41.926	1.00 1.00	72.85
	5600	CA	ALA D	126	35.472	34.595	41.450	1.00	95.10
	5601	СВ	ALA D	126	34.290	33.791	40.991	1.00	95.10 132.03
	5602	С	ALA D	126	35.119	35.403	42.693	1.00	95.10
10	5603	0	ALA D	126	35.153	34.869	43.802	1.00	95.10
10	5604	N.	LEU D	127	34.782	36.678	42.531	1.00	64.20
	5605	CA	LEU D	127	34.470	37.522	43.697	1.00	64.20
	5606	CB	LEU D	127	35.559	38.566	43.919	1.00	89.10
	5607 5608	CG CD1	LEU D	127	35.546	38.957	15.392	1.00	89.10
15	5609	CD2	LEU D	127	35.768	37.691	46.219	1.00	89.10
13	5610	C	LEU D	127 127	36.612 33.138	39.988	+5.686	1.00	89.10
	5611	ŏ	LEU D	127	32.408	38.237 38.098	43.722	1.00	64.20
	5612	N	LYS D	128	32.859	39.041	44.686	1.00	64.20
	5613	CA	LYS D	128	31.584	39.742	42.702 42.583	1.00 1.00	63.83
20	5614	CB	LYS D	128	31.737	41.203	43.000	1.00	63.83
	5615	CG	LYS D	128	32.165	41.409	44.431	1.00	126.01 126.01
	5616	CD	LYS D	128	31.058	41.080	45.416	1.00	126.01
	5617	CE	LYS D	128	31.491	41.410	46.843	1.00	126.01
25	5618	NZ	LYS D	128	30.404	₫1.252	47.855	1.00	126.01
25	5619	Ç	LYS D	128	31.160	39.675	41.109	1.00	63.83
	5620	0	LYS D	128	32.021	39.580	40.219	1.00	63.83
	5621 5622	N CA	TYR D	129	29.857	39.741	40.833	1.00	62.64
	5623	CA CB	TYR D TYR D	129	29.387	39.683	39.444	1.00	62.64
30	5624	CG	TYR D TYR D	129 129	28.984	38.268	39.098	1.00	80.75
50	5625	CD1	TYR D	129	28.046 28.521	38.200	37.928	1.00	80.75
	5626	CE1	TYR D	129	27.652	38.321 38.296	36.629 35.533	1.00	80.75
	5627	CD2	TYR D	129	26.682	38.057	38.118	1.00 1.00	80.75
	5628	CE2	TYR D	129	25.803	38.042	37.037	1.00	80.75 80.75
35	5629	CZ	TYR D	129	26.288	38.160	35.741	1.00	80.75
	5630	ОН	TYR D	129	25.412	38.145	34.662	1.00	80.75
	5631	C	TYR D	129	28.192	40.564	39.182	1.00	62.64
	5632	0	TYR D	129	27.268	40.602	39.996	1.00	62.64
40	5633	N	TRP D	130	28.190	41.252	38.042	1.00	93.45
40	5634 5635	CA	TRP D	130	27.076	42.123	37.680	1.00	93.45
	5636	CB CG	TRP D	130	27.356	43.561	38.092	1.00	113.53
	5637	CD2	TRP D	130 130	27.799 27.020	43.749	39.506	1.00	113.53
	5638	CE2	TRP D	130	27.863	44.284 44.336	40.583	1.00	113.53
45	5639	CE3	TRP D	130	25.690	44.716	41.718 40.700	1.00 1.00	113.53
	5640	CD1	TRP D	130	29.043	43.512	40.700	1.00	113.53 113.53
	5641	NE1	TRP D	130	29.092	43.864	41.347	1.00	113.53
	5642	CZ2	TRP D	130	27.413	44.811	42.961	1.00	113.53
50	5643	CZ3	TRP D	130	25.242	45.191	41.945	1.00	113.53
50	5644	CH2	TRP D	130	26.104	45.238	43.051	1.00	113.53
	5645	C	TRP D	130	26.817	42.119	36.181	1.00	93.45
	5646 5647	0	TRP D	130	27.643	41.649	35.404	1.00	93.45
	5648	N CA	TYR D	131	25.667	42.650	35.773	1.00	68.85
55	5649	CB	TYR D TYR D	131	25.343	42.732	34.351	1.00	68.8 5
-	5650	CG	TYR D	131 131	23.835 23.515	42.746 42.570	34.119	1.00	129.65
	5651	CD1	TYR D	131	23.660	42.570 41.330	32.657 32.046	1.00	129.65
	5652	CE1	TYR D	131	23.494	41.183	30.685	1.00	129.65
	5653	CD2	TYR D	131	23.182	43.661	31.862	1.00 1.00	129.65
60	5654	CE2	TYR D	131	23.015	43.523	30.495	1.00	129.65 129.65
	5655	CZ	TYR D	131	23.177	42.282	29.915	1.00	129.65
	5656	ОН	TYR D	131	23.056	42.154	28.555	1.00	129.65
	5657	Ç	TYR D	131	25.953	44.035	33.846	1.00	68.85
65	5658	0	TYR D	131	27.035	44.028	33.249	1.00	68.85
O.J	5659	N	GLU D	132	25.234	45.142	34.045	1.00	110.47
	5660 5661	CA CB	GLU D	132	25.761	46.455	33.684	1.00	110.47
	5662	CB	GLU D	132	24.715	47.569	33.878	1.00	169.41
	5663	CD	GLU D	132 132	23.632	47.688	32.798	1.00	169.41
70	5664	OE1	GLU D	132	23.679 24.276	49.022	32.059	1.00	169.41
-			D	102	L7.E/0	49.981	32.594	1.00	169.41

	5665	OE2	GLU D	132	23.107	49.114	30.951	1.00	405.44
	5666	Č	GLU D	132	26.765	46.491		1.00	169.41
	5667	ŏ	GLU D	132	26.391	46.249	34.814	1.00	110.47
	5668	Ň·	ASN D	133			35.965	1.00	110.47
5	5669	ČA	ASN D		28.029	46.777	34.515	1.00	115.67
3	5670			133	29.030	48.736	35.574	1.00	115.67
		CB	ASN D	133	30.448	46.807	35.003	1.00	113.79
	5671	CG	ASN D	133	30.911	48.198	34.814	1.00	113.79
	5672	OD1	ASN D	133	30.200	49.009	34.233	1.00	113.79
	5673	ND2	ASN D	133	32.110	48.501	35.296	1.00	113.79
10	5674	С	ASN D	133	28.888	47.723	36.718	1.00	
	5675	0	ASN D	133	28.054	48.618	36.717	1.00	115.67
	5676	N	HIS D	134	29.747	47.518	37.702		115.67
	5677	CA	HIS D	134	29.748			1.00	133.45
	5678	СВ	HIS D			48.283	38.921	1.00	133.45
15	5679	CG		134	29.100	47.430	40.006	1.00	207.58
13	5680		HIS D	134	28.893	48.141	41.302	1.00	207.58
		CD2	HIS D	134	29.411	47.919	42.534	1.00	207.58
	5681	ND1	HIS D	134	28.039	49.213	41.435	1.00	207.58
	5682	CE1	HIS D	134	28.038	49.620	42.690	1.00	207.58
	5683	NE2	HIS D	134	28.862	48.851	43.378	1.00	207.58
20	5684	С	HIS D	134	31.188	48.609	39.290	1.00	133.45
	5685	0	HIS D	134	32.09;	48.473	38.469	1.00	
	5686	N	ASN D	135	31.388	49.015	40.537	1.00	133.45
	5687	CA	ASN D	135	32.701	49.394		1.00	73.71
	5688	СВ	ASN D	135	32.877		41.017	1.00	73.71
25	5689	CG	ASN D		32.0//	50.923	40.922	1.00	127.04
23	5690		ASN D	135	32.913	51.402	39.490	1.00	127.04
		OD1	ASN D	135	33.606	50.790	38.668	1.00	127.04
	5691	ND2	ASN D	135	32.193	52.478	39.170	1.00	127.04
	5692	Ç	ASN D	135	32.869	48.930	42.441	1.00	73.71
20	5693	0	ASN D	135	32.604	49.672	43.363	1.00	73.71
30	5694	N	ILE D	136	33.307	47.689	42.606	1.00	72.93
	5695	CA	ILE D	136	33.534	47.094	43.918	1.00	72.93
	5696	CB	ILE D	136	34.435	45.852	43.786	1.00	
	5697	CG2	ILE D	136	35.652	46.164	42.961	1.00	89.30
	5698	CG1	ILE D	136	34.828	45.348		1.00	89.30
35	5699	CD1	ILE D	136			45.159	1.00	89.30
-	5700	c.			35.595	44.057	45.088	1.00	89.30
	5701			136	34.139	48.097	44.892	1.00	72.93
		O.	ILE D	136	35.241	48.602	44.689	1.00	72.93
	5702	N	SER D	137	33.393	48.393	45.952	1.00	72.75
40	5703	CA	SER D	137	33.810	49.378	46.952	1.00	72.75
40	5704	CB	SER D	137	32.797	50.514	46.982	1.00	69.16
	5705	OG	SER D	137	32.966	51.300	48.135	1.00	69.16
	5706	С	SER D	137	33.965	48.811	48.356	1.00	72.75
	5707	0	SER D	137	33.227	47.922	48.765	1.00	
	5708	Ň	ILE D	138	34.914	49.348			72.75
45	5709	CA	ILE D	138	35.171		49.106	1.00	112.14
	5710	CB	ILE D			48.888	50.464	1.00	112.14
	5711			138	36.436	48.063	50.515	1.00	65.89
		CG2	ILE D	138	36.827	47.824	51.962	1.00	65.89
	5712	CG1	ILE D	138	36.239	46.759	49.745	1.00	65.89
50	5713	CD1	ILE D	138	37.523	46.004	49.492	1.00	65.89
50	5714	С	ILE D	138	35. 359	50.050	51.431	1.00	112.14
	5715	0	ILE D	138	36.253	50.879	51.244	1.00	112.14
	5716	N	THR D	139	34.544	50.092	52.483	1.00	70.90
	5717	CA	THR D	139	34.628	51.172	53.464	1.00	
	5718	СВ	THR D	139	33.330	51.276	54. 253		70.90
55	5719	OG1	THR D	139	32.988			1.00	212.07
	5720	CG2	ם האד			49.984	<i>54.771</i>	1.00	212.07
	5721		TUD D	139	32.212	51.772	53.352	1.00	212.07
		C	THR D	139	35.791	50.913	54.409	1.00	70.90
	5722	0	THR D	139	36.851	51.523	54.280	1.00	70.90
60	5723	N	ASN D	140	35.586	50.005	55.356	1.00	80.70
OU	5724	CA	ASN D	140	36.606	49.640	56.333	1.00	80.70
	5725	CB	ASN D	140	35.957	49.206	57.644	1.00	232.63
	5726	CG	ASN D	140	36.967	48.690	58.636	1.00	232.63
	5727	OD1	ASN D	140	37.818	47.864	58.318	1.00	232.63
	5728	ND2	ASN D	140	38.862	49.170			
65	5729	C	ASN D	140	37.344		59.865 55.700	1.00	232.63
	5730	ŏ	ASN D	140		48.464	55.709	1.00	80.70
	5731	Ň			36.732	47.447	55.411	1.00	80.70
	5732	ČA	ALA D	141	38.650	48.593	55.503	1.00	77.89
			ALA D	141	39.428	47.522	54.870	1.00	77.89
70	5733 5734	CB	ALA D	141	40.437	48.086	53.919	1.00	47.27
70	5734	С	ALA D	141	40.142	46.600	55.822	1.00	77.89
								_	

	5735	0	ALA D	141	40.885	47.017	56.703	1.00	77.89
	5736	N	THR D	142	39.941	45.317	55.606	1.00	73.90
	5737	CA	THR D	142	40.557	44.300	56.434	1.00	_
	5738	CB	THR D	142	39.702	43.013	56.412	1.00	73.90
5	5739	OG1	THR D	142	38.346	43.343	56.745		158.80
	5740	CG2	THR D	142				1.00	158.80
					40.214	42.014	57.416	1.00	158.80
	5741	C	THR D	142	41.927	44.055	55.837	1.00	73.90
	5742	0	THR D	142	42.236	44.606	54.779	1.00	73.90
• •	5743	N	VAL D	143	42.756	43.268	56.521	1.00	104.07
10	5744	CA	VAL D	143	44.088	42.953	56.008	1.00	104.07
	5745	CB	VAL D	143	45.093	42.610	57.127	1.00	127.52
	5746	CG1	VAL D	143	44.701	41.320	57.807	1.00	
	5747	CG2	VAL D	143	46.495	42.479	56.545	1.00	127.52
	5748	C	VAL D	143	43.955	41.736			127.52
15	5749	ŏ	VAL D	143			55.107	1.00	104.07
1.5	5750	Ň			44.846	41.424	54.322	1.00	104.07
			GLU D	144	42.829	41.046	55.222	1.00	87.28
	5751	CA	GLU D	144	42.603	39.874	54.400	1.00	87.28
	5752	СВ	GLU D	144	41.492	39.011	55.003	1.00	215.80
00	5753	CG	GLU D	144	41.840	38.428	56.363	1.00	215.80
20	5754	CD	GLU D	144	40.992	39.001	57.475	1.00	215.80
	5755	OE1	GLU D	144	39.756	38.856	57.409	1.00	215.80
	5756	OE2	GLU D	144	41.555	39.596	58.416	1.00	
	5757	C	GLU D	144	42.245	40.287	52.982	1.00	215.80
	5758	ŏ	GLU D	144	42.288	39.478			87.28
25	5759	Ň	ASP D				52.074	1.00	87.28
25				-#45 45	41.898	41.556	52.801	1.00	67.03
	5760	CA	ASP D		41.533	42.083	51.491	1.00	67.03
	5761	CB	ASP D	145	40.847	43.441	51.634	1.00	129.44
	5762	CG	ASP D	145	39.448	43.320	52.163	1.00	129.44
20	5763	OD1	ASP D	145	38.636	42.636	51.510	1.00	129,44
30	5764	OD2	ASP D	145	39.158	43.899	53.228	1.00	129,44
	5765	С	ASP D	145	42.751	42.217	50.587	1.00	67.03
	5766	0	ASP D	145	42.634	42.396	49.365	1.00	67.03
	5767	N	SER D	146	43.932	42.121	51.177	1.00	89.85
	5768	CA	SER D	146	45.140	42.235	50.383	1.00	89.85
35	5769	C8	SER D	146	46.366	42.277	51.300	1.00	212.33
	5770	OG	SER D	146	46.317	43.408	52,152	1.00	212.33
	5771	C	SER D	146	45.185	41.034	49.452	1.00	
	5772	ŏ	SER D	146	44.810	39.933			89.85
	5773	Ň	GLY D	147	45.604	41.256	49.836	1.00	89.85
40	5774	ČA	GLY D	147			48.213	1.00	67.51
-10	5775	Č.	GLY D		45.698	40.164	47.254	1.00	67.51
				147	46.000	40.693	45.865	1.00	67.51
	5776	0	GLY D	147	46.475	41.825	45.724	1.00	67.51
	5777	N	THR D	148	45.740	39.888	44.835	1.00	62.13
45	5778	CA	THR D	148	45.975	40.327	43.454	1.00	62.13
43	5779	CB	THR D	148	47.073	39.493	42.770	1.00	85.2°
	5780	OG1	THR D	148	46.483	38.564	41.871	1.00	85.26
	5781	CG2	THR D	148	47.863	38,729	43.800	1.00	85.26
	5782	С	THR D	148	44.665	40.210	42.689	1.00	62.13
	5783	0	THR D	148	44,106	39.134	42.527	1.00	62.13
50	5784	N	TYR D	149	44.164	41.339	42.230	1.00	42.52
	5785	CA	TYR D	149	42.894	41.349	41.547	1.00	42.52
	5786	СВ	TYR D	149	42.072	42.518	42.079		
	5787	CG	T /O 0					1.00	42.86
	57 83	CD1	TYP D	149	41.722	42.498	43.543	1.00	42.86
55	5789	CE1	TYR D	149	42.689	42.662	44.522	1.00	42.86
<i>J J</i>			TYR D	149	42.339	42.702	45.880	1.00	42.86
	5790	CD2	TYR D	149	40.404	42.373	43.936	1.00	42.86
	5791	CE2	TYR D	149	40.038	42.412	45.251	1.00	42.86
	5792	CZ	TYR D	149	40.998	42.570	46.237	1.00	42.86
<i>(</i> 0	5793	OH	TYR D	149	40.592	42.542	47.568	1.00	42.86
60	5794	С	TYR D	149	43.028	41.506	40.046	1.00	42.52
	5795	0	TYR D	149	44.102	41.847	39.556	1.00	42.52
	5796	N	TYR D	150	41.921	41.262	39.340	1.00	57.99
	5797	CA	TYR D	150	41.799	41.429	37.892	1.00	57.99
	5798	СВ	TYR D	150	42.675	40.420	37.108	1.00	88.00
65	5799	CG	TYR D	150	42.197	38.986			
-	5800	CD1	TYR D	150	41.124	38.661	36.975 36.156	1.00	00.88
	5801	CE1	TYR D	150	40.693			1.00	88.00
	5802	CD2	TYR D	150	42.840	37. 3 42	36.010	1.00	88.00
	5803	CE2	TYR D			37.948	37.649	1.00	88.00
70	5804	CZ	TYR D	150	42.422	36.626	37.513	1.00	88.00
	JUU-1	· ·	ITH D	150	41.342	36.327	36.692	1.00	88.00

	5805	OH	TYR D	150	40.898	35.020	36.578	1.00	88.00
	5806	Ç	TYR D	150	40.293	41.260	37.623	1.00	57.99
	5807	0	TYR D	150	39.569	40.702	38.470	1.00	57.99
5	5808	N	CYS D	151	39.793	41.782	36.500	1.00	62_97
J	5809	CA C	CYS D	151	38.365	41.650 41.175	36.193	1.00	62.97
	5810 5811	Ö	CYS D	151 151	38.136 39.009	41.175 41.229	34.780 33.931	1.00	62.97
	5812	СВ	CYS D	151	37.636	42.966	36.413	1.00 1.00	62.97
	5813	SG	CYS D	151	38.287	44.417	35.527	1.00	102.16
10	5814	Ň	THR D	152	36.975	40.566	34.538	1.00	102.16 73.20
	5815	CA	THR D	152	36.613	40.055	33.215	1.00	73.20
	5816	СВ	THR D	152	36.437	38.527	33.230	1.00	136.00
	5817	OG1	THR D	152	35.288	38.183	34.017	1.00	136.00
	5818	CG2	THR D	152	37.664	37.855	33.814	1.00	136.00
15	5819	С	THR D	152	35.286	40.688	32.830	1.00	73.20
	5820	0	THR D	152	34.434	40.945	33.698	1.00	73.20
	5821	N	GLY D	153	35.105	40.950	31.538	1.00	64.84
	5822	CA	GLY D	153	33.863	41.572	31.099	1.00	64.84
20	5823 5824	c o	GLY D	153	33.682	41.463	29.609	1.00	64.84
20	5825	N	GLY D	153 154	34.636 32.462	41.184 41.680	28.899	1.00	64.84
	5826	CA	LYS D	154	32.180	41.576	29.133 27.706	1.00	72.61
	5827	CB	LYS D	154	30.881	40.800	27.706	1.00 1.00	72.61
	5828	CG	LYS D	154	30.546	40.515	26.030	1.00	205.73 205.73
25	5829	CD	LYS D	154	29.274	39.697	25.956	1.00	205.73
	5830	CE	LYS D	154	C2 825	39.439	24.533	1.00	205.73
	5831	NZ	LYS D	154	27.516	38.730	24.533	1.00	205.73
	5832	C	LYS D	154	32.056	42.967	27.134	1.00	72.61
••	5833	0	LYS D	154	31.329	43.802	27.662	1.00	72.61
30	5834	N	VAL D	155	32.792	43.226	26.065	1.00	92.93
	5835	CA	VAL D	155	32.751	44.532	25.426	1.00	92.93
	5836	CB	VAL D	155	34.140	45.153	25.313	1.00	130.27
	5837	CG1 CG2	VAL D	155	34.065	46.494	24.609	1.00	130.27
35	5838 5839	C	VAL D	· 155 155	34.714	45.331	26.689	1.00	130.27
33	5840	ŏ	VAL D	155	32.216 32.715	44.275 43.395	24.040 23.330	1.00	92.93
	5841	Ň	TRP D	156	31.205	45.046	23.653	1.00 1.00	92.93 158.38
	5842	ČA	TRP D	156	30.579	44.860	22,358	1.00	158.38
	5843	CB	TRP D	156	31.605	44.866	21.235	1.00	243.82
40	5844	CG	TRP D	156	32.236	46.155	21.100	1.00	243.82
	5845	CD2	TRP D	156	31.589	47.366	20.812	1.00	243.82
	5846	CE2	TRP D	156	32.575	48.376	20.781	1.00	243.82
	5847	CE3	TRP D	156	30.261	47.713	20.608	1.00	243.82
45	5848	CD1	TRP D	156	33.550	46.428	21.198	1.00	243.82
43	5849	NE1	TRP D	156	33.771	47.767	21.014	1.00	243.82
	5850 5851	CZ2 CZ3	TRP D	156	32.278	49.703	20.533	1.00	243.82
	5852	CH2	TRP D	156 156	29.993 30.983	49.006	20.358	1.00	243.82
	5853	C	TRP D	156	29.982	49.997 43.492	20.320 22.407	1.00	243.82
50	5854	ŏ	TRP D	156	28.886	43.299	22.908	1.00 1.00	158.38 158.38
	5855	Ň	GLN D	157	30.752	42.528	21.924	1.00	148.04
	5856	CA	GLN D	157	30.284	41.168	21.881	1.00	148.04
	5857	CB	GLN D	157	29.612	40.948	20.533	1.00	249.45
	5858	CG	GLN D	157	28.288	41.684	20.483	1.00	249.45
55	5859	CD	GLN D	157	27.435	41.306	21.676	1.00	249.45
	5860	OE1	JIN D	157	27.203	40.132	21.914	1.00	249.45
	5861	NE2	GLN D	157	26.963	42.292	22.421	1.00	249.45
	5862	C	GLN D	157	31.348	40.127	22.150	1.00	148.04
60	5863 5864	O N	GLN D LEU D	157	31.140	38.936	21.912	1.00	148.04
00	5865	CA	LEU D	158	32.488	40.579	22.665	1.00	85.54
	5866	CB	LEU D	158 158	33.584 34.779	39.676 39.917	22.996 22.073	1.00	85.54 127.62
	5867	ČG	LEU D	158	34.714	39.361	22.073 20.649	1.00 1.00	127.62 127.62
Δ	5868	CD1	LEU D	158	36.094	38.823	20.329	1.00	127.62
65	5869	CD2	LEU D	158	33.694	38.231	20.514	1.00	127.62
	5870	C	LEU. D	158	34.022	39.797	24.457	1.00	85.54
	5871	0	LEU D	158	33.857	40.847	25.090	1.00	85.54
	5872	N	ASP D	159	34.562	38.706	24.986	1.00	91.88
70	5873	CA	ASP D	159	35.024	38.662	26.363	1.00	91.88
70	5874	CB	ASP D	159	34.915	37.229	26.901	1.00	249.49

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	5875	CG CD1	ASP D	159	33.518	36.644	26.743	1.00	249.49
	5876	OD1	ASP D	159	32.559	37.204	27.319	1.00	249.49
	5877	OD2	ASP D	159	33.380	35.620	26.039	1.00	249.49
_	5878	C	ASP D	159	36.476	39.142	26.462	1.00	91.88
5	5879	0	ASP D	159	37.270	38.921	25.543	1.00	91.88
	5880	N	TYR D	160	36.818	39.807	27.568	1.00	90.02
	5881	CA	TYR D	160	38.179	40.298	27.785	1.00	90.02
	5882	СВ	TYR D	160	38.334	41.742	27.323	1.00	132.54
	5883	ÇG	TYR D	160	37.907	41.996	25.905	1.00	132.54
10	5884	CD1	TYR D	160	36.605	42.362	25.617	1.00	132.54
	5885	CE1	TYR D	160	36.196	42.585	24.315	1.00	132.54
	5886	CD2	TYR D	160	38.800	41.857	24.851	1.00	
	5887	CE2	TYR D	160	38.405	42.075	23.539	1.00	132.54
	5888	CZ	TYR D	160	37,101	42.437	23.278		132.54
15	5889	OH	TYR D					1.00	132.54
13	5890			160	36.697	42.638	21.977	1.00	132.54
		C	TYR D	160	38.594	40.222	29.239	1.00	90.02
	5891	0	TYR D	160	37.782	40.394	30.143	1.00	90.02
	5892	N.	GLU D	161	39.884	39.979	29.436	1.00	92.36
20	5893	CA	GLU D	161	40.492	39.862	30.750	1.00	92.36
20	5894	CB	GLU D	161	41.247	38.536	30.815	1.00	148.75
	5895	CG	GLU D	161	42.005	38.266	32.084	1.00	148.75
	5896	CD	GLU D	161	42,398	36.810	32.189	1.00	148.75
	5897	OE1	GLU D	161	43.333	36.490	32.957	1.00	148.75
	5898	OE2	GLU D	161	41.757	35.985	31.506	1.00	148.75
25	5899	С	GLU D	161	41.448	41.051	30.923	1.00	92.36
	5900	0	GLU D	161	42.157	41.424	29.985	1.00	92.36
	5901	N	SER D	162	41.450	41.655	32.110	1.00	74.96
	5902	CA	SER D	162	42.323	42.789	32,404	1.00	
	5903	CB	SER D	162	41.652	43.705			74.96
30	5904	OG OB	SER D	162	41.377	42.998	33.398	1.00	62.82
50	5905	Č	SER D			42.370	34.594	1.00	62.82
	5906	ŏ		162	43.671		32.989	1.00	74.96
			SER D	162	43.876	41.208	33.354	1.00	74.96
	5907	N	GLU D	163	44.593	43.325	33.088	1.00	68.26
35	5908	CA	GLU D	163	45.929	43.034	33.625	1.00	68.26
33	5909	CB	GLU D	163	46.877	44.206	33.368	1.00	242.79
	5910	ÇG	GLU D	163	47.352	44.338	31.925	1.00	242.79
	5911	CD	GLU D	163	48.358	43.266	31.540	1.00	242.79
	5912	OE1	GLU D	163	49.400	43.158	32,222	1.00	242.79
40	5913	OE2	GLU D	163	48.113	42.537	30.556	1.00	242.79
40	5914	С	GLU D	163	45.768	42.820	35.117	1.00	68.26
	5915	0	GLU D	163	44.970	43.504	35.751	1.00	68.26
	5916	N	PRO D	164	46.511	41.863	35.698	1.00	51.48
	5917	CD	PRO D	164	47.539	40.983	35.148	1.00	112.85
	5918	CA	PRO D	164	46.359	41.659	37.137	1.00	51.48
45	5919	СВ	PRO D	164	47.112	40.364	37.367	1.00	112.85
	5920	ČĠ	PRO D	164	48.211	40.465	36.404		
	5921	č	PRO D	164	46.955	42.827	37.920	1.00	112.85
	5922	ŏ	PRO D	164	47.839			1.00	51.48
	5923	Ň	LEU D	165		43.536	37.411	1.00	51.48
50	5924	CA			46.480	43.045	39.145	1.00	58.03
50	5925			165	46.988	44.134	39.944	1.00	58.03
		CB	LEU D	165	46.085	45.333	39.824	1.00	67.82
	5926	CG	LEU D	165	46.417	46.436	40.816	1.00	67.82
	5927	CD1	LEU D	165	47.878	46.685	40.736	1.00	67.82
EE	5928	CD2	LEU D	165	45.653	47.711	40.495	1.00	67.82
55	5929	С	LEU D	165	47.080	43.744	41.384	1.00	58.03
	5930	0	LEU D	165	46.082	43.313	41.957	1.00	58.03
	5931	N	ASN D	166	48.274	43.892	41.964	1.00	50.98
	5932	CA	ASN D	166	48.513	43.551	43.367	1.00	50.98
	5933	CB	ASN D	166	49.984	43.249	43.618	1.00	110.65
60	5934	CG	ASN D	166	50.324	41,777	43.461	1.00	110.65
	5935	OD1	ASN D	166	49.514	40.900	43.700		
	5936	ND2	ASN D	166	51.557	41.517	43.077	1.00	110.65
	5937	C	ASN D	166	48.084			1.00	110.65
	5938	ŏ	ASN D			44.660	44.311	1.00	50.98
65	5939	N		166	48.175	45.818	43.992	1.00	50.98
05	5940			167	47.626	44.290	45.489	1.00	69.36
		CA	ILE D	167	47.167	45.267	46.443	1.00	69.36
	5941	CB	ILE D	167	45.659	45.375	46.397	1.00	42.00
	5942	CG2	ILE D	167	45.152	46.062	47.661	1.00	42.00
70	5943	CG1	ILE D	167	45.241	46.105	45.129	1.00	42.00
70	5944	CD1	ILE D	167	43.748	46.402	45.115	1.00	42.00

	5945	С	11.5	407	47.500				
	5946	ŏ	ILE D	167 167	47.557 47.366	44.842 43.682	47.833 48.218	1.00	69.36
	5947	N	THR D	168	48.090	45.774	48.603	1.00 1.00	69.36 69.22
5	5948	CA.	THR D	168	48.480	45.418	49.945	1.00	69.22
3	5949	CB	THR D	168	49.988	45.453	50.107	1.00	70.81
	5950 5951	OG1 CG2	THR D THR D	168	50.575	44.544	49.169	1.00	70.81
	5952	C	THR D	168 168	50.372 47,8₄∶	45.030 46.301	51.511	1.00	70.81
	5953	Ö	THR D	168	47.754	47.509	50.987 50.828	1.00 1.00	69.22
10	5954	N	VAL D	169	47.387	45.670	52.051	1.00	69.22 66.57
	5955	CA	VAL D	169	46.774	46.361	53.155	1.00	66.57
	5956 5957	CB CG1	VAL D VAL D	169	45.379	45.806	53.417	1.00	62.74
	5958	CG2	VAL D	169 169	44.945 44.418	46.137 46.381	54.819	1.00	62.74
15	5959	c	VAL D	169	47.693	46.061	52.416 54.334	1.00 1.00	62.74
	5960	0	VAL D	169	47.740	44.932	54.805	1.00	66.57 66.57
	5961	N	ILE D	170	48.460	47.051	54.780	1.00	82.22
	5962 5963	CA CB	ILE D	170	49.360	46.864	55.913	1.00	82.22
20	5964	CG2	ILE D	170 170	50.599 51.201	47.738	55.759	1.00	114.31
	5965	CG1	ILE D	170	50.232	47.504 49.218	54.406	1.00	114.31
	5966	CD1	ILE D	170	51.416	50.187	55. 860 55. 670	1.00 1.00	114.31
	5967	Ç	ILE D	170	48.613	47.237	57.189	1.00	114.31 82.22
25	5968	0	ILE D	170	47.459	47.676	57.122	1.00	82.22
23	5969 5970	N CA	LYS D	171	49.245	47.053	58.347	1.00	108.79
	5971	CB	LYS D LYS D	171 171	48.598 48.214	47.390	59.620	1.00	108.79
	5972	CG	LYS D	171	49.380	46.117 45.194	60.360 60.614	1.00	188.56
20	5973	CD	LYS D	171	48.910	43.762	60.800	1.00 1.00	188.56 188.56
30	5974	CE	LYS D	171	47.946	43.624	61.976	1.00	188.56
	5975 5976	NZ	LYS D	171	47.459	42.220	62.130	1.00	188.56
	5977	C	LYS D LYS D	171 171	49.453	48.270	60.524	1.00	108.79
	5978	Č1	NAG D	221	48.981 40.344	48.761 65.6 2 9	61.549	1.00	108.79
35	5979	C2	NAG D	221	39.010	64.922	28.022 27.810	1.00 1.00	249.77
	5980	N2	NAG D	221	39.203	63.489	27.903	1.00	249.77 249.77
	5981	C7	NAG D	221	38.191	62.705	28.261	1.00	249.77
	5982 5983	O7 C8	NAG D NAG D	221	37.073	63.139	28.545	1.00	249.77
40	5984	$\ddot{\mathbf{g}}$	NAG D	221 221	38.462 38.434	61.211 65.256	28.324	1.00	249.77
	5985	03	NAG D	221	37.116	64.735	26.441 26.342	1.00 1.00	249.77
	5986	C4	NAG D	221	38.404	66.763	26.173	1.00	249.77 249.77
	5987	04	NAG D	221	38.077	66.947	24.777	1.00	249.77
45	5988 5989	C5 O5	NAG D NAG D	221	39.780	67.394	26.498	1.00	249.77
	5990	C6	NAG D	221 221	40.191 39.770	67.042 68.913	27.838	1.00	249.77
	5991	06	NAG D	221	38.854	69.459	26.439 27.379	1.00 1.00	249.77
	5992	C1	NAG D	222	37.635	68.189	24.343	1.00	249.77 233.91
50	5993 5994	C2	NAG D	222	36.436	68.019	23.396	1.00	233.91
50	599 4 5995	N2 C7	NAG D	222	35.346	67.346	24.082	1.00	233.91
	5996	07	nag d Nag d	222 222	34.173 33.947	67.955	24.234	1.00	233.91
	5997	C8	NAG D	222	33.082	69.093 67.183	23.816 24.963	1.00	233.91
	5998	C3	NAG D	222	36.855	67.215	22.156	1.00 1.00	233.91 233.91
55	5999	03	NAG D	222	35.790	67.196	21.217	1.00	233.91
	6000 6001	C4	NAG D	222	38.102	67.829	21.503	1.00	.91
	6002	O4 C5	nag d Nag d	222 222	38.567	66.974	20.471	1.00	233.91
	6003	O5	NAG D	222	39.211 38.722	68.020 68.817	22.542	1.00	233.91
60	6004	C6	NAG D	222	40.435	68.722	23.644 21.989	1.00 1.00	233.91
	6005	Q6	NAG D	222	41.628	68.076	22.406	1.00	233.91 233.91
	6006	C1	NAG D	242	59.627	58.578	32.960	1.00	107.57
	6007 6008	C2 N2	NAG D	242	59.450	58.871	31.486	1.00	107.57
65	6009	C7	NAG D NAG D	242 242	59.010	60.232	31.316	1.00	107.57
	6010	07	NAG D	242 242	59.707 60.732	61.044 60.679	30.534	1.00	107.57
	6011	C8	NAG D	242	59.199	62.478	29.950 30.373	1.00 1.00	107.57
	6012	C3	NAG D	242	58.412	57.932	30.887	1.00	107.57 107.57
70	6013	O3	NAG D	242	58.316	58.138	29.483	1.00	107.57
, 0	6014	C4	NAG D	242	58.806	56.496	31.148	1.00	107.57

e:

	8015	04	NAO D	0.40					
	6015 6016	O4 C5	NAG D NAG D	24 <u>2</u> 242	57.728	55.629	30.752	1.00	107.57
	6017	O5	NAG D	242	59.118 60.064	56.268 57.236	32.625	1.00	107.57
	6018	C6 .	NAG D	242	59.783	54.930	33.114 32.783	1.00	107.57
5	6019	06	NAG D	242	59.082	54.107	33.697	1.00 1.00	107.57
	6020	C1	NAG D	243	57.985	54.762	29.705	1.00	107.57
	6021	C2	NAG D	243	57.074	53.527	29.789	1.00	125.30 125.30
	6022	N2	NAG D	243	57.321	52.782	31.013	1.00	125.30
10	6023	C7	NAG D	243	56.303	52.357	31.758	1.00	125.30
10	6024	07	NAG D	243	55.129	52.583	31.473	1.00	125.30
	6025	C8	NAG D	243	56.634	51.574	33.018	- 1.00	125.30
	6026 6027	C3 O3	NAG D	243	57.345	52.629	28.586	1.00	125.30
	6028	C4	NAG D NAG D	243 243	56.458	51.521	28.595	1.00	125.30
15	3029	04	NAG D	243	57.191 57.612	53.414 52.582	27.277	1.00	125.30
	6030	C5	NAG D	243	58.083	54.659	26.156 27.339	1.00	125.30
	6031	O5	NAG D	243	57.744	55.459	28.483	1.00 1.00	125.30
	6032	C6	NAG D	243	57.985	55.549	26.119	1.00	125.30 125.30
-	6033	O6	NAG D	243	56.713	56.172	26.043	1.00	125.30
20	6034	C1	MAN D	244	56.846	52.424	25.031	1.00	205.85
	6035	C2	MAN D	244	55.417	51.844	25.171	1.00	205.85
	6036	02	MAN D	244	54.487	52.897	25.184	1.00	205.85
	6037 6038	C3	MAN D	244	55.275	51.012	23.858	1.00	205.85
25	6039	O3 C4	MAN D MAN D	244	54.016	50.380	23.757	1.00	205.85
20	6040	04	MAN D	244 244	55.586 55.419	51.831	22.569	1.00	205.85
	6041	C5	MAN D	244	57.054	51.015 52.305	21.411	1.00	205.85
	6042	O 5	MAN D	244	57.244	53.154	22.669 23.833	1.00 1.00	205.85
••	6043	C6	MAN D	244	57.597	52.991	21.412	1.00	205.85 205.85
30	6044	O6	MAN D	244	57.221	54.349	21.357	1.00	205.85
	6045	C1	NAG D	250	45.992	76.510	37.679	1.00	248.68
	6046	C2	NAG D	250	44.579	76.931	. 38.128	1.00	248.68
	6047 6048	N2	NAG D	250	44.536	77.116	39.567	1.00	248.68
35	6049	C7 O7	NAG D NAG D	250	44.384	78.333	40.083	1.00	248.68
-	6050	C8	NAG D	250 250	44.277 44.348	79.347	39.391	1.00	248.68
	6051	Č3	NAG D	250	43.573	78.442 75.849	41.599	1.00	248.68
	6052	03	NAG D	250	42.252	76.265	37.715 38.034	1.00 1.00	248.68
40	6053	C4	NAG D	250	43.682	75.570	36.213	1.00	248.68 248.68
40	6054	04	NAG D	250	42.841	74.477	35.869	1.00	248.68
	6055	C5	NAG D	250	45.139	75.244	35.834	1.00	248.68
	6056	O5	NAG D	250	46.017	76.312	36.259	1.00	248.68
	6057 6058	C6 . O6	NAG D	250	45.335	75.070	34.335	1.00	248.68
45	6059	. 06 C1	NAG D NAG D	250	46.713	75.089	33.986	1.00	248.68
15	6060	C2	NAG D	274 274	63.247 62.953	69.025	55.540	1.00	209.92
	6061	N2	NAG D	274	61.768	68.056 68.477	56.695	1.00	209.92
	6062	C7	NAG D	274	61.053	67.585	57.416 58.098	1.00 1.00	209.92
	6063	07	NAG D	274	61.342	66.390	58.145	1.00	209.92 209.92
50	6064	C8	NAG D	274	59.826	68.096	58.835	1.00	209.92
	6065	C3	NAG D	274	64.147	68.007	57.654	1.00	209.92
•	6066	03	NAG D	274	63.927	67.009	58.639	1.00	209.92
	6067	C4	NAG D	274	65.443	67.703	56.893	1.00	209.92
55	6068 6069	O4 C5	NAG D	274	66.552	67.817	57.775	1.00	209.92
55	6070	O5	NAG D	274	65.610	68.683	55.725	1.00	209.92
	6071	C6	NAG D	274 274	64.452 66.820	68,631	54.865	1.00	209.92
	6072	06	NAG D	274	66.810	68.373 69.142	54.862 53.667	1.00	209.92
	6073	C1	NAG D	335	32.860	53.594	38.525	1.00 1.00	209.92
60	6074	C2	NAG D	335	32.657	54.924	39.281	1.00	187.23 187.23
	6075	N2	NAG D	335	32.302	54.604	40.651	1.00	187.23
	6076	C7	NAG D	335	33.089	54.970	41.656	1.00	187.23
	6077	07	NAG D	335	34.133	55.601	41.498	1.00	187.23
65	6078	C8	NAG D	335	32.640	54.583	43.054	1.00	187.23
J	6079 6080	C3	NAG D	335	31.561	55.826	38.691	1.00	187.23
	6081	O3 C4	NAG D	335	31.736	57.155	39.169	1.00	187.23
	6082	⊙ 4	NAG D NAG D	335 335	31.606	55.833 56.616	37.168	1.00	187.23
	6083	C5	NAG D	335	30.534 31.498	56.616 54.394	36.658 36.658	1.00	187.23
70	6084	O5	NAG D	335	32.666	53.657	36.668 37.089	1.00	187.23
•					500		37.003	1.00	187.23

	6085	C6	NAC D	005	04.440	54.047			
	6086	O6	NAG D NAG D	335 335	31.442 30.243	54.317 53.705	35.144 34.692	1.00	187.23
	6087	C1	NAG D	340	36.447	48.280	60.935	1.00 1.00	187.23
	6088	C2 ·	NAG D	340	37.563	48.157	61.941	1.00	247.88
5	6089	N2	NAG D	340	38.786	47.736	61.296	1.00	247.88 247.88
	6090	C7	NAG D	340	39.907	48.420	61.502	1.00	247.88
	6091	07	NAG D	340	39.959	49.402	62.248	1.00	247.88
	6092 6093	C8 C3	NAG D	340	41.160	47.954	60.781	1.00	247.88
10	6094	⊙ ⊙3	NAG D NAG D	340 340	37.180 38.213	47.173	63.025	1.00	247.88
	6095	C4	NAG D	340	35.881	47.101 47.637	64.002 63.677	1.00 1.00	247.88
	6096	04	NAG D	340	35.406	46.605	64.547	1.00	247.88
	6097	C5	NAG D	340	34.778	47.988	62.613	1.00	247.88 247.88
	6098	O5	NAG D	340	35.305	48.810	61.587	1.00	247.88
15	6099	C6	NAG D	340	33.729	48.850	63.239	1.00	247.88
	6100	O6	NAG D	340	33.003	49.565	62.297	1.00	247.88
	6101 6102	C1 C2	NAG D NAG D	366	51.975	40.156	42.859	1.00	179.92
	6103	N2	NAG D	366 366	53.015 52.433	40.152 40.714	41.753 40.551	1.00 1.00	179.92
20	6104	C7	NAG D	366	52.553	42.013	40.303	1.00	179.92 179.92
	6105	07	NAG D	366	53.160	42.786	41.048	1.00	179.92
	6106	C8	NAG D	366	51.908	42.532	39.029	1.00	179.92
	6107	C3	NAG D	366	53.483	38.733	41.488	1.00	179.92
25	6108	03	NAG D	366	54.558	38.758	40.562	1.00	179.92
25	6109 6110	C4 O4	NAG D NAG D	366 366	53.939	38.053	42.783	1.00	179.92
	6111	C5.	NAG D	366	54.150 52.883	36.651 38.216	42.516	1.00	179.92
	6112	O5	NAG D	366	52.522	39.602	43.899 44.056	1.00 1.00	179.92
	6113	C6	NAG D	366	53.364	37.740	45.257	1.00	179.92 179.92
30	6114	O 6	NAG D	366	52.346	37.880	46.242	1.00	179.92
	6115	C1	NAG D	367	55.386	36.120	42.861	1.00	249.52
	6116	C2	NAG D	367	55.270	34.606	43.041	1.00	249.52
	6117 6118	N2 C7	NAG D NAG D	367	54.288	34.289	44.061	1.00	249.52
35	6119	07 07	NAG D	367 367	53.121 52.823	33.757 33.510	43.710	1.00	249.52
	6120	C8	NAG D	367	52.132	33.450	42.539 44.8 2 5	1.00 1.00	249.52 249.52
	6121	ca	NAG D	367	56.643	34.041	43.413	1.00	249.52
	6122	03	NAG D	367	56.568	32.629	43.535	1.00	249.52
40	6123	C4	NAG D	367	57.655	34.411	42.327	1.00	249.52
40	6124 6125	O4 C5	NAG D	367	58.951	33.973	42.709	1.00	249.52
	6126	O5	NAG D NAG D	367 367	57.659 56.321	35.931 36.405	42.108	1.00	249.52
	6127	C6	NAG D	367	58.553	36.343	41.807 40.953	1.00 1.00	249.52
	6128	O6	NAG D	367	57.795	36.836	39.858	1.00	249.52 249.52
45	6129	CB	LYS E	4	12.130	63.790	1.727	1.00	181.25
	6130	ca	LYS E	4	10.709	63.348	1.434	1.00	181.25
	6131 6132	CD	LYS E	4	9.964	63.056	2.721	1.00	181.25
	6133	CE NZ	LYS E LYS E	4	8.534 7.791	62.631	2.447	1.00	181.25
50	6134	C	LYS E	4	12.157	62.349 65.259	3.709 -0.281	1.00	181.25
	6135	ŏ	LYS E	4	11.355	65.991	0.294	1.00 1.00	249.30 249.30
	6136	N	LYS E	4	14.286	64.661	0.874	1.00	249.30
	6137	CA	LYS E	4	12.924	64.186	0.485	1.00	249.30
55	6138	N	PRO E	5	12.400	65.365	-1.597	1.00	120.68
23	6139 6140	CD CA	PRO E	5	13.529	64.775	-2.329	1.00	144.78
	6141	CB	PRO E PRO E	5 5	11.713	66.365 66.600	-2.422	1.00	120.68
	6142	ČĠ	PRO E	5	12.699 13.298	66.600 65.263	-3.566	1.00	144.78
	6143	C	PRO E	5	10.345	65.902	-3.751 -2.912	1.00 1.00	144.78 120.68
60	6144	0	PRO E	5	10.065	64.705	-2.963	1.00	120.68
	6145	N	LYS E	6	9.489	66.856	-3.263	1.00	141.31
	6146	CA	LYS E	6	8.153	66.534	-3.743	1.00	141.31
	6147	CB	LYS E	6	7.152	66.622	-2.590	1.00	196.63
65	6148 6149	CD	LYS E Lys e	6	5.747	66.182	-2.959	1.00	196.63
-5	6150	CE	LYS E	6 6	4.834 3.443	66.110 65.623	-1.741	1.00	196.63
	6151	NZ	LYS E	6	2.521	65.453	-2.137 -0.973	1.00	196.63
	6152	С	LYS E	6	7.735	67.460	-0.973 -4.883	1.00 1.00	196.63 141.31
70	6153	0	LYS E	6	7.596	68.669	-4.698	1.00	141.31
70	6154	N	VAL E	7	7.526	66.874	-6.059	1.00	81.07
						•			

	6155 6156 6157	CA CB CG1	VAL E VAL E VAL E	7. 7 7	7.145 7.188 6.965	67.622 68.745 67.610	-7.259 -8.530 -9.757	1.00	81.07 76.53
5	6158 6159	CG2 C	VAL E	7 7	8.488 5.738	66,003 68,181	-9.757 -8.626 -7.212	1.00	76.53 76.53
	6160 6161	O N .	VAL E SER E	7 8	4.778 5.606	67.426 69.498	-7.151 -7.268	1.00 1.00 1.00	81.07 81.07
	6162 6163	CA CB	SER E SER E	8	4.287 4.268	70.111 71.325	-7.266 -6.332	1.00	146.33 146.33
10	6164 6165	OG C	SER E SER E	8 8	5.288 3.948	72.253 70.536	-6.669 -8.692	1.00 1.00 1.00	208.51 208.51
	6166 6167	O N	SER E LEU E	8 9	4.829 2.671	70.605 70.806	-9.548 -8.946	1.00 1.00 1.00	146.33 146.33
15	6168 6169	CA CB	LEU E	9	2.221 1.358	71.236 70.166	-10.269 -10.929	1.00	130.86 130.86
	6170 6171	CG CD1	LEU E	9	1.921	68.783 68.115	-10.929 -11.217 -12.291	1.00	129.83 129.83
	6172 6173	CD2 C	LEU E	9	3.337 1.393	68.911 72.513	-11.693	1.00	129.83 129.83
20	6174 6175	0 N	LEU E ASN E	9 10	0.783	72.822	-10.206 -9.184	1.00	130.86 130.86
	6176 6177	CA CB	ASN E ASN E	10	1.356 0.572	73.248 74.473	-11.311 -11.372	1.00 1.00	238.98 238.98
25	6178 6179	. CG OD1	ASN E ASN E	10 10	1.327 0.451	75.629 76.844	-10.726 -10.530	1.00 1.00	166.05 166.05
2,5	6180 6181	ND2	ASN E	10 10	-0.489 0.745	76.822 77.911	-9.737 -11.263	1.00 1.00	166.05 166.05
	6182	0	ASN E ASN E	10 10	0.235 1.112	74.821 75.191	-12.817 -13.598	1.00 1.00	238.98 238.98
30	6183 6184	N CD	PRO E	11 11	-1.053 -1.439	74.715 74.939	-13.195 -14.595	1.00 1.00	125.56 163.67
	6185 6186	CA CB	PRO E	11 11	-2.214 -3.341	74.304 74.258	-12.392 -13.429	1.00 1.00	125.56 163.67
35	6187 6188	CG C	PRO E	11	-2.903 -2.053	75.247 72.952	-14.467 -11.676	1.00 1.00	163.67 125.56
23	6189 6190	0	PRO E	11 12	-1.179 -2.887	72.163 72.668	-12.027 -10.663	1.00 1.00	125.56 68.14
	6191 6192	CD CA	PRO E	12 12	-3.978 -2.8 2 6	73.517 71.412	-10.138 -9.907	1.00 1.00	156.84 68.14
40	6193 6194	CB CG	PRO E	12 12	-3.863 -4.037	71.600 73.077	-8.802 -8.709	1.00 1.00	156.84 156.84
	6195 6196	0 2	PRO E	12 12	-3.214 -2.835	70.234 69.084	-10.814 -10.562	1.00 1.00	68.14 68.14
45	6197 6198	N CA	TRP E	13 13	-3.987 -4.488	70.547 69.551	-11.857 -12.800	1.00 1.00	90.03 90.03
43	6199 6200	CB CG	TRP E	13 13	-5.267 -6.235	70.231 71.215	-13.916 -13.407	1.00 1.00	120.89 120.89
	6201 6202	CD2 CE2	TRP E	13 13	-7.024 -7.750	71.111 72.310	-12.227 -12.102	1.00 1.00	120,89 120,89
50	6203 6204	CE3 CD1	TRP E	13 13	-7.191 -6.509	70.121 72.430	-11.255 -13.945	1.00 1.00	120.89 120.89
	6205 6206	NE1 CZ2	TRP E	13 13	-7.418 -8.627	73.100 72.548	-13,167 -11.042	1.00 1.00	120.89 120.89
55	6207 6208	CZ3 CH2	TRP E	13 13	-8.065 -8.768	70.359 71.561	-10.204 -10.104	1.00 1.00	120.89 120.89
55	6209 6210	С 0	TRP E	13 13	-3.377 -2.479	68.727 69.264	-13.398 -14.031	1.00 1.00	90.03 90.03
	6211 6212	N CA	ASN E ASN E	14 14	-3.443 -2.431	67.415 66.516	-13.192 -13.720	1.00 1.00	80.76 80.76
60	6213 6214	CB CG	ASN E ASN E	14 14	-1.883 -2.896	65.579 64.571	-12.622 -12.133	1.00 1.00	101.28 101.28
	6215 6216	OD1 ND2	ASN E ASN E	14 14	-3.979 -2.542	64.933 63.293	-11.674 -12.211	1.00 1.00	101.28 101.28
<i>(</i>	6217 6218	C	ASN E ASN E	14 14	-2.917 -2.303	65.715 64.709	-14.921 -15.288	1.00 1.00	80.76 80.76
65	6219 6220	N CA	ARG E ARG E	15 15	-4.026 -4.554	66.154 65.520	-15.523 -16.732	1.00	74.26 74.26
	6221 6222	CB CG	ARG E ARG E	15 15	-5.855 -5.888	64.779 63.996	-16.490 -15.236	1.00	82.67 82.67
70	6223 6224	CD NE	ARG E ARG E	15 15	-7.202 -7.314	63.278 62.199	-15.142 -16.114	1.00 1.00	82.67 82.67
								-	

	6225	CZ	ARG E	15	-8.470	61.801	-16.627	1.00	82.67
	6226	NH1	ARG E	15	-9.582	62.415	-16.260	1.00	82.67
	6227	NH2	ARG E	15	-8.523	60.784	-17.483	1.00	82.67
5	6228	C .	ARG E	15	-4.860	66.730	-17.570	1.00	74.26
)	6229	0	ARG E	15	-5.753	67.509	-17.232	1.00	74.26
	6230 6231	N CA	ILE E	16	-4.116	66.920	-18.647	1.00	117.86
	6232	CA CB	ILE E	16	-4.363	68.085	-19.460	1.00	117.86
	6233	CG2	ILE E	16 16	-3.213	69.070 69.663	19.378	1.00	89.68
10	6234	CG1	ILE E	16	-3.128 -1.917	68.359	-17.980 -19.758	1.00	89.68
	6235	CD1	ILE E	16	-0.707	69.252	-19.676	1.00 1.00	89.68
	6236	Č.	ILE E	16	-4.589	67.773	-20.909	1.00	89.68
	6237	ō	ILE E	16	-4.302	66.678	-21.390	1.00	117.86 117.86
	6238	N	PHE E	17	-5.103	68.784	-21.591	1.00	150.96
15	6239	CA	PHE E	17	-5.417	68.746	-23.003	1.00	150.96
	6240	CB	PHE E	17	-6.466	69.815	-23.287	1.00	92.59
	6241	CG	PHE E	17	-7.872	69.337	-23.168	1.00	92.59
	6242	CD1	PHE E	17	-8.846	70.151	-22.597	1.00	92.59
20	6243	CD2	PHE E	17	-8.251	68.120	-23.724	1.00	92.59
20	6244	CE1	PHE E	17	-10.193	69.757	-22.577	1.00	92.59
	6245	CE2	PHE E	17	-9.588	67.717	-23.711	1.00	92.59
	6246 6247	CZ C	PHE E	17	-10.567	68.546	-23.141	1.00	92.59
	6248	ŏ	PHE E	17	-4.169	69.021	-23.835	1.00	150.96
25	6249	Ň	LYS E	17 18	-3.184 -4.222	69.562 68.665	-23.333	1.00	150.96
	6250	ČA	LYS E	18	-3.099	68.891	-25.112 -26.010	1.00	145.64
	6251	CB	LYS E	18	-3.370	68.206	-27.350	1.00 1.00	145.64
	6252	CG	LYS E	18	-2.210	68.241	-28.329	1.00	192.00
	6253	CD	LYS E	18	-2.457	67.244	-29.441	1.00	192.00 192.00
30	6254	CE	LYS E	18	-1.359	67.245	-30.495	1.00	192.00
	6255	NZ	LYS E	18	-1.218	68.567	-31.165	1.00	192.00
	6256	С	LYS E	18	-2.878	70.388	-26.224	1.00	145.64
	6257	0	LYS E	18	-3.814	71.129	-26.517	1.00	145.64
25	6258	N	GLY E	19	-1.638	70.835	-26.061	1.00	249.22
35	6259	CA	GLY E	19	-1.339	72.237	-26.278	1.00	249.22
	6260	C	GLY E	19	-1.364	73.144	-25.065	1.00	249.22
	6261 6262	0 N	GLY E	19	-0.954	74.298	-25.156	1.00	249.22
	6263	CA	GLU E	20	-1.837	72.648	-23.930	1.00	144.61
40	6264	CB	GLU E	20 20	-1.882 -2.930	73.481 72.929	-22.732	1.00	144.61
	6265	CG	GLU E	20	-4.288	72.690	-21.759 -22.425	1.00	147.82
	6266	CD	GLU E	20	-5.371	72.050 72.257	-22.425 -21.449	1.00 1.00	147.82 147.82
	6267	OE1	GLU E	20	-5.166	71.259	-20.729	1.00	147.82
	6268	OE2	GLU E	20	-6.435	72.910	-21.411	1.00	147.82
45	6269··	С	GLU E	20	-0.501	73.546	-22.071	1.00	144.61
	6270	0	GLU E	20	0.412	72.815	-22.466	1.00	144.61
	6271	N	ASN E	21	-0.335	74.432	-21.089	1.00	165.65
	6272	CA	ASN E	21	0.951	74.549	-20.407	1.00	165.65
50	6273	CB	ASN E	21	1.551	75.953	-20.547	1.00	216.79
30	6274	CG	ASN E	21	1.361	76.551	-21.918	1.00	216.79
	6275 6276	OD1	ASN E	21	1.528	75.886	-22.943	1.00	216.79
	6277	ND2 C	ASN E ASN E	21	1.027	77.836	-21.921	1.00	216.79
	6278	ŏ	ASN E	21 21	0.837	74.248	-18.917	1.00	165.65
55	6279	Ň	VAL E	22	-0.147 1.868	74.602 73.608	-18.268 -18.380	1.00	165.65
	6280	CA	VAL E	22	1.912	73.265	-16.968	1.00 1.00	160.77
	6281	CB	VAL E	22	1.497	71.820	-16.737	1.00	160.77 158.92
	6282	CG1	VAL E	22	2.481	70.881	-17.426	1.00	158.92
	6283	CG2	VAL E	22	1.448	71.543	-15.256	1.00	158.92
60	6284	С	VAL E	22	3.342	73.442	-16.467	1.00	160.77
	6285	0	VAL E	22	4.306	73.287	-17.229	1.00	160.77
	6286	N	THR E	23	3.478	73.743	-15.180	1.00	119.61
	6287	CA	THR E	23	4.789	73.972	-14.581	1.00	119.61
65	6288	CB	THR E	23	4.862	75.412	-14.037	1.00	249.32
UJ	6289	OG1	THR E	23	4.505	76.335	-15.075	1.00	249.32
	6290 6291	CG2	THR E	23	6.255	75.728	-13.537	1.00	249.32
	6292	C	THR E	23	5.089	73.004	-13.434	1.00	119.61
	6293	N	THR E LEU E	23 24	4.291	72.881 72.226	-12.515	1.00	119.61
70	6294	CA	LEU E	24	6.233 6.556	72.326 71.397	-13.467	1.00	105.17
					0.330	11.387	-12.387	1.00	105.17

	6295	СВ	LEU E	24	7.032	70.045	-12.922	1.00	144.47
	6296	CG	LEU E	24	6.394	69.466	-14.178	1.00	144.47
	6297	CD1	LEU E	24	6.782	68.008 69.607	-14.314 -14.118	1.00 1.00	144.47 144.47
5	6298	CD2	LEU E	24 24	4.904 7.635	71.944	-11.482	1.00	105.17
2	6299	C	LEU E	24	8.814	71.943	-11.821	1.00	105.17
	6300 6301	N	THR E	25	7.238	72.386	-10.306	1.00	95.95
	6302	ČA	THR E	25	8.206	72.926	-9.380	1.00	95.95
	6303	CB	THR E	25	7.552	74.012	-8.528	1.00	178.12
10	6304	OG1	THR E	25	6.961	74.986	-9.397	1.00	178.12
	6305	CG2	THR E	25	8.578	74.689	-7.639	1.00	178.12
	6306	Ç	THR E	25	8.786	71.833	-8.486 -8.004	1.00 1.00	95.95 05.95
	6307	0	THR E	25	8.062 10.098	70.964 71.858	-8.279	1.00	95.95 175.10
15	6308	N CA	CYS E CYS E	26 26	10.709	70.859	-7.421	1.00	175.10
13	6309 6310	CA	CYS E	26	10.708	71.335	-5.991	1.00	175.10
	6311	ŏ	CYS E	26	10.769	72.518	-5.698	1.00	175.10
	6312	СВ	CYS E	26	12.178	70.637	-7.771	1.00	230.60
	6313	SG	CYS E	26	12.906	69.220	-6.890	1.00	230.60
20	6314	N	ASN E	27	10.293	70.392	-5.114	1.00	159.04
	6315	CA	ASN E	27	10.141	70.641	-3.696	1.00	159.04
	6316	CB	ASN E	27	10.980	69.628 69.486	-2.940 -1.511	1.00 1.00	118.85 118.85
	6317	CG	ASN E	27 27	10.546 9.351	69.537	-1.211	1.00	118.85
25	6318 6319	OD1 ND2	ASN E	27	11.506	69.298	-0.613	1.00	118.85
23	6320	C	ASN E	27	10.502	72.054	-3.237	1.00	159.04
	6321	ŏ	ASN E	27	11.646	72.331	-2.882	1.00	159.04
	6322	Ň	GLY E	28	9.516	72.944	-3.238	1.00	225.84
	6323	CA	GLY E	28	9.750	74.315	-2.824	1.00	225.84
30	6324	С	GLY E	28	8.487	75.101	-3.091	1.00	225.84
	6325	0	GLY E	28	8.021	75.153	-4.227 -2.059	1.00 1.00	225.84 249.43
	6326	N	ASN E ASN E	29 29	7.929 6.693	75.722 76.466	-2.228	1.00	249.43
	6327	CA CB	ASN E	29	6.026	76.682	-0.870	1.00	249.43
35	6328 6329	CG	ASN E	29	4.607	77.193	-0.996	1.00	249.43
33	6330	OD1	ASN E	29	3.999	77.145	-2.066	1.00	249.43
	6331	ND2	ASN E	29	4.067	77.674	0.104	1.00	249.43
	6332	С	ASN E	29	6.820	77.799	-2.962	1.00	249.43
40	6333	0	ASN E	29	6.084	78.052	-3.920 -2.530	1.00	249.43
40	6334	N	ASN E	30	7.746 7.903	78.649 79.952	·2.530 ·3.169	1.00 1.00	249.58 249.58
	6335	CA	ASN E ASN E	30 30	7.903 7.420	81.060	-2.229	1.00	249.27
	6336 6337	CB	ASN E	30	5.941	80.965	-1.929	1.00	249.27
	6338	OD1	ASN E	30	5.532	80.984	-0.770	1.00	249.27
45	6339	ND2	ASN E	30	5.128	80.865	-2.974	1.00	249.27
••	6340	C	ASN E	30	9.313	80.279	-3.633	1.00	249.58
	6341	0	ASN E	30	9.589	80,313	-4.833	1.00	249.58
	6342	N	PHE E	31	10.206	80.526	-2.682	1.00	249.39 249.39
50	6343	CA	PHE E	31	11.567 11.939	80.882 82.212	-3.038 -2.368	1.00 1.00	249.59 249.51
50	6344	CB	PHE E	31 31	10.976	83.336	-2.673	1.00	249.51
	6345 6346	CG CD1	PHE E	31	9.760	83.431	-2.003	1.00	249.51
	6347	CD2	PHE E	31	11.275	84.285	-3.649	1.00	249.51
	6348	CE1	PHE E	31	8.855	84.455	-2.294	1.00	249.51
55	6349	CE2	PHE E	31	10.278	85.313	-3.949	1.00	249.51
	6350	CZ	PHE E	31	9.164	85.396	-3.270	1.00	249.51
	6351	Ç	PHE E	31	12.602	79.806	-2.729	1.00	249.39
	6352	0	PHE E	31	12.696	79.305	-1.605	1.00	249.39 249.36
60	6353	N	PHE E	32 32	13.374	79.462 78.447	-3.760 -3.678	1.00 1.00	249.36
OU	6354 6355	CA CB	PHE E PHE E	32	14.421 14.088	77.296	-4.623	1.00	231.13
	6356	CG	PHE E	32	14.910	76.075	-4.386	1.00	231.13
	6357	CD1	PHE E	32	14.771	75.366	-3.200	1.00	231.13
	6358	CD2	PHE E	32	15.844	75.644	-5.325	1.00	231.13
65	6359	CE1	PHE E	32	15.547	74.245	-2.944	1.00	231.13
	6360	CE2	PHE E	32	16.628	74.520	-5.079	1.00	231.13
	6361	CZ	PHE E	32	16.477	73.819	-3.881	1.00	231.13
	6362	C	PHE E	32	15.779	79.040	-4.063 -4.540	1.00	249.36 249.36
70	6363	.O N	GLU E	32 33	15.849 16.857	80.171 78. <i>2</i> 77	-4.540 -3.876	1.00 1.00	249.36 249.65
70	6364	M	GLU E	30	10.007	.10.211	0.070	1.00	270.00

	6365	CA	GLU E	33	18.190	78.784	-4.212	1.00	249.65
	6366	CB	GLU E	33	19.035	78.993	-2.958	1.00	249.51
	6367	CG	GLU E	33	20.347	79.715	-3.258	1.00	249.51
	6368	CD .	GLU E	33	20.106	81.122	-3.769	1.00	249.51
5	6369	OE1	GLU E	33	19.170	81.769	-3.253	1.00	249.51
_	6370	OE2	GLU E	33	20.849	81.591	-4.659	1.00	
	6371	C	GLU E	33	19.038	77.975	-5.180		249.51
		ŏ						1.00	249.65
	6372		GLU E	33	19.533	78.510	-6.173	1.00	249.65
10	6373	N	VAL E	34	19.242	76.699	-4.873	1.00	249.34
10	6374	CA	VAL E	34	20.073	75.864	-5.721	1.00	249.34
	6375	CB	VAL E	34	20.055	74.399	-5.244	1.00	177.29
	6376	CG1	VAL E	34	20.927	73.540	-6.146	1.00	177.29
	6377	CG2	VAL E	34	20.562	74.325	-3.815	1.00	177.29
	6378	C	VAL E	34	19.694	75.933	-7.196	1.00	
15		ŏ							249.34
13	6379		VAL E	34	18.530	76.142	-7.555	1.00	249.34
	6380	N	SER E	35	20.705	75.782	-8.040	1.00	249.49
	6381	CA	SER E	35	20.523	75.809	-9.479	1.00	249.49
	6382	CB	SER E	35	21.517	76.779	-10.122	1.00	217.44
	6383	OG	SER E	35	22.845	73.294	-10.006	1.00	217.44
20	6384	С	SER E	35	20.763	74.397	-10.001	1.00	249.49
	6385	õ	SER E	35.	20.658	74,144	-11.199	1.00	249.49
	6386	Ň	SER E	36					
			SER E		21.094	73.480	-9.092	1.00	249.36
	6387	CA	SER E	36	21.335	72.089	-9.464	1.00	249.36
~ =	6388	CB	SER E	36	22.586	71.540	-8.769	1.00	172.90
25	6389	OG	SER E	36	22.371	71.370	-7.379	1.00	172.90
	6390	С	SER E	36	20.128	71.242	-9.085	1.00	249.36
	6391	0	SER E	36	20.020	70.741	-7.964	1.00	249.36
	6392	Ň	THR E	37	19.214	71.104	-10.036	1.00	210.16
	6393	CA	THR E	37					
30					18.007	70.321	-9.849	1.00	210.16
30	6394	CB	THR E	37	16.754	71.225	-9.905	1.00	202.55
	6395	OG1	THR E	37	16.859	72.253	-8.913	1.00	202.55
	6396	CG2	THR E	37	15.499	70.414	-9.647	1.00	202.55
	6397	С	THR E	37	17.982	69.325	-11.000	1.00	210.16
	6398	0	THR E	37	18.352	69.662	-12.126	1.00	210.16
35	6399	N	LYS E	38	17.565	68.098	-10.718	1.00	223.06
	6400	CA	LYS E	38	17.517	67.070	-11.749	1.00	223.06
	6401	CB	LYS E						
				38	18.234	65.818	-11.256	1.00	249.17
	6402	CG	LYS E	38	19.660	66.069	-10.828	1.00	249.17
40	6403	CD	LYS E	38	20.313	64.794	-10.338	1.00	249.17
40	6404	CE	LYS E	38	21.769	65.032	-9.996	1.00	249.17
	6405	NZ	LYS E	38	22.436	63.783	-9.543	1.00	249.17
	6406	С	LYS E	38	16.086	66.711	-12.133	1.00	223.06
	6407	O	LYS E	38	15.204	66.678	-11.281	1.00	223.06
	6408	Ň	TRP E	39	15.858	66.451	-13.418	1.00	178.64
45	6409	CA	TRP E						
73				39	14.530	66.068	-13.895	1.00	178.64
	6410	CB	TRP E	39	13.911	67.160	-14.768	1.00	178.88
	6411	CG	TRP E	39	13.622	68.431	-14.049	1.00	178.88
	6412	CD2	TRP E	39	12.634	68.651	-13.034	1.00	178.88
	6413	CE2	TRP E	39	12.721	70.008	-12.652	1.00	178.88
50	6414	CE3	TRP E	39	11.685	67.832	-12.407	1.00	178.88
	6415	CD1	TRP E	39	14.249	69.627	-14.235	1.00	178.88
	6416	NE1	TRP E	39	13.712	70.580	-13.400	1.00	
	6417	CZ2		39		70.564			178.88
					11.896		-11.678	1.00	178.88
<i>E E</i>	6418	CZ3	TRP E	39	10.865	68.390	-11.436	1.00	178.88
55	6419 ,	CH2	TRP E	39	10.978	69.744	-11.081	1.00	178.88
	6420	С	TRP E	39	14.641	64.796	-14.710	1.00	178.64
	6421	0	TRP E	39	15.495	64.687	-15.582	1.00	178.64
	6422	N	PHE E	40	13.771	63.838	-14.432	1.00	223.76
	6423	CA	PHE E	40	13.811	62.585	-15.159	1.00	223.76
60	6424	CB	PHE E	40	14.209	61.445	-14.223	1.00	
00			DUE E						188.15
	6425	CG	PHE E	40	15.514	61.660	-13.529	1.00	188.15
	6426	CD1	PHE E	40	15.592	62.472	-12.407	1.00	188.15
	6427	CD2	PHE E	40	16.663	61.029	-13.984	1.00	188.15
	6428	CE1	PHE E	40	16.797	62.656	-11.746	1.00	188.15
65	6429	CE2	PHE E	40	17.875	61.204	-13.333	1.00	188.15
	6430	CZ	PHE E	40	17.942	62.020	-12.207	1.00	188.15
	6431	Č_	PHE E	40	12.490	62.235	-15.834	1.00	223.76
	6432	ŏ	PHE E						
				40	11.665	61.521	-15.266	1.00	223.76
70	6433	N	HIS E	41	12.294	62.737	-17.048	1.00	123.84
70	6434	CA	HIS E	41	11.080	62.448	-17.801	1.00	123.84

	C40E	СВ	LUC E	41	10.940	63,454	-18.937	1.00	104.40
	6435		HIS E						124.43
	6436	CG	HIS E	41	9.749	63.222	-19.801	1.00	124.43
	6437	CD2	HIS E	41	9.597	63.290	-21.144	1.00	124.43
	6438	ND1	HIS E	41	8.510	62.907	-19.289	1.00	124.43
5			1110 C						
)	6439	CE1	HIS E	41	7.645	62.789	-20.278	1.00	124.43
	6440	NE2	HIS E	41	8.280	63.016	-21.415	1.00	124.43
	6441	С	HIS E	41	11.136	61.013	-18.349	1.00	123.84
	6442	ŏ	HIS E	41	11.924	60.715	-19.243	1.00	123.84
	6443	N	ASN E	42	10.298	60.132	-17.809	1.00	190.21
10	6444	CA	ASN E	42	10.269	58.717	-18.206	1.00	190.21
	6445	CB	ASN E	42	10.027	58.550	-19.720	1.00	194.75
	6446	ČĞ	ASN E	42	8.588	58.839	-20.123	1.00	194.75
	6447	OD1	ASN E	42	8.009	59.813	-19.653	1.00	194.75
	6448	ND2	ASN E	42	8.017	58.019	-21.005	1.00	194.75
15	6449	С	ASN E	42	11.593	58.050	-17.826	1.00	190.21
		ŏ	ASN E	42	12.003	57.072	-18.446	1.00	190.21
	6450								
	6451	N	GLY E	43	12.263	58.580	-16.806	1.00	203.91
	6452	$ abla \Delta$	GLY E	43	13.533	58.010	-16.386	1.00	203.91
	6453	C	GLY E	43	14.734	58.697	-17.020	1.00	203.91
20						58.901		1.00	
20	6454	0		43	15.758		-16.364		203.91
	6455	N	SER E	44	14.609	59.053	-18.297	1.00	245.20
	6456	CA	SER E	44	15.683	59.723	-19.030	1.00	245.20
	6457	CB	SER E	44	15.312	59.846	-20.512	1.00	220.02
~ ~	6458	OG	SER É	44	14.940	58.591	-21.055	1.00	220.02
25	6459	С	SER E	44	15.929	61.114	-18.452	1.00	245,20
	6460	0	SER E	44	14.999	61.907	-18.326	1.00	245.20
	6461	Ň	LEU F	45	17.177	61.412	-18.101	1.00	174.49
	6462	CA	LEU E	45	17.519	62.718	-17.541	1.00	174.49
	6463	CB	LEU E	45	19.028	62.804	-17.280	1.00	249.38
30	6464	CG	LEU E	45	19.550	64.104	-16.660	1.00	249.38
-	6465	CD1	LEU E	45	18.785	64.404	-15.381	1.00	249.38
	6466	CD2	LEU E	45	21.043	63.982	-16.375	1.00	249.38
	6467	С	LEU E	45	17.095	63.834	-18.498	1.00	174.49
	6468	0	LEU E	45	17.140	63.672	-19.717	1.00	174.49
35	6469	Ň	SER E	46	16.673	64.965	-17.945	1.00	153.34
"									
	6470	CA	SER E	46	16.247	66.094	-18.766	1.00	153.34
	6471	CB	SER E	46	15.016	66.766	-18.148	1.00	249.33
	6472	OG	SER E	46	14.541	67.822	-18.971	1.00	249.33
	6473	Č	SER E	46	17.394	67.088	-18.845	1.00	153.34
40								1.00	
40	6474	0	SER E	46	18.345	66.994	-18.072		153.34
	6475	N	GLU E	47	17.310	68.043	-19.768	1.00	221.85
	6476	CA	GLU E	47	18.371	69.035	-19.903	1.00	221.85
	6477	CB	GLU E	47	18.589	69.401	-21.384	1.00	249.45
						68.232	-22,369	1.00	249.45
4 ~	6478	CG	GLU E	47	18.515				
45	6479	CD	GLU E	47	18.351	68.687	-23.823	1.00	249.45
	6480	OE1	GLU E	47	17.207	68.973	-24.239	1.00	249.45
	6481	OE2	GLU E	47	19.372	68.774	-24.540	1.00	249.45
			GLU E					1.00	
	6482	Ç		47	18.128	70.317	-19.081		221.85
	6483	0	GLU E	47	18.974	71.207	-19.091	1.00	221.85
50	6484	N	GLU E	48	16.993	70.438	-18.387	1.00	204.14
	6485	CA	GLU E	48	16.775	71.643	-17.573	1.00	204.14
			GLU E	48		71.939	-17.355	1.00	206.52
	6486	CB		40	15.275				
	6487	CG	GLU E	48	14.973	73.087	-16.352	1.00	206.52
	6488	CD	GLU E	48	15.418	74.469	-16.P <i>2</i> 3	1.00	206.52
55	6489	OE1	GLU I	48	14.812	74.995	-17.778	1.00	206.52
55									206.52
	6490	OE2	GLU E	48	16.370	75.032	-16.236	1.00	
	6491	С	GLU E	48	17.471	71.443	-16.221	1.00	204.14
	6492	0	GLU E	48	17.724	70.311	-15.798	1.00	204.14
	6493	N	THR E	49	17.803	72.545	-15.556	1.00	206.12
60									
OU	6494	CA	THR E	49	18.472	72.476	-14.266	1.00	206.12
	6495	СВ	THR E	49	19.947	72.928	-14.386	1.00	224.40
	6496	OG1	THR E	49	20.006	74.247	-14.942	1.00	224.40
	6497	CG2	THR E	49	20.721	71.972	-15.288	1.00	224.40
CF	6498	Č	THR E	49	17.747	73.335	-13.233	1.00	206.12
65	6499	0	THR E	49	17.781	73.043	-12.035	1.00	206.12
	6500	N	ASN E	50	17.081	74.388	-13.702	1.00	231.11
	6501	CA	ASN E	50	16.330	75.272	-12.819	1.00	231.11
	6502		ASN E		15.602	76.349	-13.640		
		CB		50				1.00	176.85
	6503	CG	ASN E	50	15.085	77.491	-12.783	1.00	176.85
70	6504	OD1	ASN E	50	14.962	77.346	-11.568	1.00	176.85
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	6505	ND2	ASN E	50	14.770	78.622	-13.410	1.00	470.05
	6506	C	ASN E	50	15.316	74.396	-12.076		176.85
	6507	Ŏ	ASN E	50	14.884	73.368 ·		1.00	231.11
	6508	Ň.	SER E	51			-12.597	1.00	231.11
5	6509	ČA			14.942	74.792	-10.863	1.00	235.89
J			SER E	51	13.985	74.015	-10.077	1.00	235.89
	6510	CB	SER E	51	13.895	74.561	-8.645	1.00	153.05
	6511	OG	SER E	51	13.254	75.826	-8.609	1.00	153.05
	6512	С	SER E	51	12.587	73.995	-10.696	1.00	235.89
	6513	0	SER E	51	11.765	73.145	-10.358	1.00	
10	6514	Ń	SER E	52	12.314	74.932	-11.597		235.89
	6515	CA	SER E	52				1.00	154.90
	6516	CB			11.009	74.997	-12.245	1.00	154.90
			SER E	52	10.435	76.415	-12.157	1.00	199.68
	6517	OG	SER E	52	10.195	76.786	-10.809	1.00	199.68
1.5	6518	С	SER E	52	11.109	74.569	-13.700	1.00	154.90
15	6519	0	SER E	52	11.656	75.288	-14.538	1.00	154.90
	6520	N	LEU E	53	10.582	73.385	-13.985	1.00	
	6521	CA	LEU E	53	10,590	72.827	-15.332		130.79
	6522	СВ	LEU E	53	10.833			1.00	130.79
	6523	ČĞ	LEU E			71.315	-15.264	1.00	134.25
20	6524			53	10.394	70.457	-16.457	1.00	134,25
20		CD1	LEU E	53	10.802	71.095	-17.779	1.00	134.25
	6525	CD2	LEU E	53	10.999	69.065	-16.304	1.00	134.25
	6526	С	LEU E	53	9.271	73.112	-16.044	1.00	130.79
	6527	0	LEV E	53	8.279	72.435	-15.810	1.00	130.79
	6528	N	ASN E	54	9.258	74.109	-16.920	1.00	
25	6529	CA	ASN E	54	8.031	74.440			200.88
	6530	СВ	ASN E	54			-17.632	1.00	200.88
	6531	CG			8.095	75.864	-18.181	1.00	249.13
			ASN E	54	7.990	76.907	-17.096	1.00	249.13
	6532	OD1	ASN E	54	7.029	76.923	-16.328	1.00	249.13
20	6533	ND2	ASN E	54	8.975	77.790	-17.026	1.00	249.13
30	6534	С	ASN E	54	7.719	73.486	-18.771	1.00	200.88
	6535	0	ASN E	54	8.589	72.769	-19.265	1.00	200.88
	6536	N	ILE E	55	6.453	73.481	-19.168		
	6537	CA	ILE E	55	5.985	72.657		1.00	204.06
	6538	CB	ILE E	55			-20.269	1.00	204.06
35	6539	CG2			5.212	71.417	-19.770	1.00	202.84
55			ILE E	55	4.367	70.839	-20.896	1.00	202.84
	6540	CG1	ILE E	55	6.205	70.376	-19.246	1.00	202.84
	6541	CD1	ILE E	5 5	5.569	69.111	-18.716	1.00	202.84
	6542	С	ILE E	55	5.065	73.547	-21.080	1.00	204.06
	6543	0	ILE E	55	4.086	74.074	-20.559	1.00	204.06
40	6544	N	VAL E	56	5.395	73.739	-22.349	1.00	
	6545	CA	VAL E	56	4.580	74.585			244.52
	6546	СВ	VAL E	56			-23.202	1.00	244.52
	6547	CG1	VAL E		5.458	75.494	-24.072	1.00	219.78
	6548			56	4.629	76.643	-24.618	1.00	219.78
45		CG2	VAL E	56	6.622	76.026	-23.246	1.00	219.78
40	6549	C	VAL E	56	3.711	73.696	-24.073	1.00	244.52
	6550	0	VAL E	56	3.545	72.522	-23.758	1.00	244.52
	6551	N	ASN E	57	3.160	74.247	-25.152	1.00	153.88
	6552	CA	ASN E	57	2.290	73.486	-26,047	1.00	
	6553	CB	ASN E	57	2.564	73.854	-27.506	1.00	153.88
50	6554	CG	ASN E	57	2.105	75.254			249.23
	6555	OD1	ASN E	57			-27.843	1.00	249.23
	6556	ND2			0.954	75.617	-27.601	1.00	249.23
			ASN E	57	3.003	76.051	-28.404	1.00	249.23
	6557	Ç	ASN E	57	2.438	71.983	-25.847	1.00	153.88
	6558	0	ASN E	57	3.263	71.323	-26.489	1.00	153.88
55	6559	N	ALA E	58	1.624	71.458	-24.936	1.00	183.15
	6560	CA	ALA E	58	1.638	70.047	-24.587	1.00	
	6561	CB	ALA E	58	0.552	69.763	-23.565		183,15
	6562	C	ALA E	58	1.492			1.00	127.72
	6563	ŏ	ALA E			69.103	-25.766	1.00	183.15
60	6564		ALA E	58	0.486	69.115	-26.474	1.00	183.15
00		N	LYS E	59	2.510	68.281	-25.968	1.00	111.87
	6565	CA	LYS E	59	2.495	67. 29 3	-27.035	1.00	111.87
	6566	CB	LYS E	59	3.816	67.338	-27.815	1.00	249.40
	6567	CG	LYS E	59	4.115	68.702	-28.436	1.00	249.40
	6568	CD	LYS E	59	5.489	68.753	-29.090	1.00	
65	6569	CE	LYS E	59	5.764	70.129			249.40
	6570	NZ	LYS E	59			-29.691	1.00	249.40
	6571	C			7.117	70.219	-30.310	1.00	249.40
			LYS E	59 50	2.319	65.942	-26.334	1.00	111.87
	6572	0	LYS E	59	2.824	65.746	-25.226	1.00	111.87
70	6573	N.	PHE E	60	1.597	65.020	-26.960	1.00	223.03
70	6574	CA	PHE E	60	1.368	63.703	-26.366	1.00	223.03
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	CETE	СВ	PHE E	60	0.846	62.744	-27.427	1.00	249.06
	6575		PHE E		-0.496	63.120	-27.953	1.00	249.06
	6576	CG		60			-29.237		
	6577	CD1 _.	PHE E	60	-0.876	62.774		1.00	249.06
	6578	CD2	PHE E	60	-1.390	63.823	-27.155	1.00	249.06
5	6579	CE1	PHE E	60	-2.124	63.119	-29.727	1.00	249.06
•	6580	CE2	PHE E	60	-2.640	64.176	-27. 63 3	1.00	249.06
	6581	čz	PHE E	60	-3.010	63.822	-28.922	1.00	249.06
			PHE E	60	2.610	63.115	-25.720	1.00	223.03
	6582	Ç				62.404	-24.721	1.00	
	6583	0	PHE E	60	2.520				223.03
10	6584	N	GLU E	61	3.771	63.417	-26.296	1.00	190.77
	6585	CA	GLU E	61	5.044	62.917	-25.783	1.00	190.77
	6586	СВ	GLU E	61	6.196	63.299	-26.718	1.00	249.27
	6587	CG	GLU E	61	6.096	62.728	-28.116	1.00	249.27
		CD	GLU E	61	4.851	63.190	-28.838	1.00	249.27
15	6588				4.635	64.418	-28.924	1.00	249.27
15	6589	OE1	GLU E	61					249.27
	6590	OE2	GLU E	61	4.090	62.327	-29.320	1.00	
	6591	С	GLU E	61	5.357	63.449	-24.395	1.00	190.77
	6592	0	GLU E	61	6.140	62.842	-23.663	1.00	190.77
	6593	N	ASP E	62	4.765	64.588	-24.040	1.00	156.70
20	6594	CA	ASP E	62	5.006	65.174	-22.727	1.00	156.70
20		CB	ASP E	62	4.489	66.613	-22.678	1.00	165.21
	6595						-23.792	1.00	165.21
	6596	CG	ASP E	62	5.062	67.477			
	6597	OD1	ASP E	62	6.251	67.299	-24.133	1.00	165.21
	6598	OD2	ASP E	62	4.329	68.341	-24.320	1.00	165.21
25	6599	С	ASP E	62	4.3/1	64.324	-21.643	1.00	156.70
23	6600	ŏ	ASP E	62	4.711	64.394	-20.470	1.00	156.70
		Ň	SER E	63	3.358	63.523	-22.045	1.00	140.02
	6601				2.672	62.635	-21.118	1.00	140.02
	6602	CA	SER E	63					
	6603	СВ	SER E	63	1.618	61.796	-21.856	1.00	116.21
30	6604	OG	SER E	63	0.557	62.589	-22.368	1.00	116.21
	6605	С	SER E	63	3.744	61.710	-20.557	1.00	140.02
	6606	Ö	SER E	63	4.509	61.128	-21.315	1.00	140.02
	6607	Ň	GLY E	64	3.818	61.572	-19.243	1.00	94.90
		CA	GLY E	64	4.835	60.694	-18.698	1.00	94.90
25	6608					60.749	-17.195	1.00	94.90
35	6609	Ç	GLY E	64	5.050			1.00	
	6610	0	GLY E	64	4.252	61.333	-16.462	1.00	94.90
	6611	N	GLU E	65	6.127	60.121	-16.737	1.00	137.73
	6612	CA	GLU E	65	6.476	60.071	-15.323	1.00	137.73
	6613	CB	GLU E	65	6.875	58.635	-14.971	1.00	170.42
40	6614	CG	GLU E	65	7.492	58.437	-13.609	1.00	170.42
70		CD	GLU E	65	8.153	57.072	-13.484	1.00	170.42
	6615			65	9.121	56.807	-14.233	1.00	170.42
	6616	OE1	GLU E		3.121		-12.644	1.00	170.42
	6617	OE2	GLU E	65	7.706	56.263			
	6618	С	GLU E	65	7.645	61.025	-15.096	1.00	137.73
45	6619	0	GL' E	65	8.653	60.925	-15.789	1.00	137.73
	6620	N	TYR E	66	7.513	61.952	-14.147	1.00	117.13
	6621	CA	TYR E	66	8.588	62.908	-13.864	1.00	117.13
	6622	CB	TYR E	66	8.123	64.321	-14.112	1.00	93.74
			TYR E	66	7.767	64.647	-15.528	1.00	93.74
50	6623	CG	TIN E					1.00	93.74
50	6624	CD1	TYR E	66	6.586	64.214	-16.090		
	6625	CE1	TYR E	66	6.220	64.609	-17.382	1.00	93.74
	6626	CD2	TYR E	66	8.582	65.471	-16.285	1.00	93.74
	6627	CE2	TYR E	66	8.230	65.873	-17.564	1.00	93.74
	6628	CZ	TYR E	66	7.050	65.445	-18.110	1.00	93.74
55	6629	OH OH	TYR E	66	6.702	65.872	-19.376	1.00	93.74
33			TYR E	66	9.062	62.852	-12.426	1.00	117.13
	6630	Ç						1.00	117.13
	6831	0	TYR E	66	8.359	62.335	-11.564		
	6632	N	LYS E	67	10.248	63.402	-12.169	1.00	125.36
	6633	CA	LYS E	67	10.802	63.443	-10.815	1.00	125.36
60	6634	CB	LYS E	67	11.186	62.037	-10.352	1.00	181.51
	6635	ÇĞ	LYS E	67	12.026	61.282	-11.345	1.00	181,51
	6636	CD	LYS E	67	12.264	59.876	-10.876	1.00	181.51
						59.066	-11.956	1.00	181.51
	6637	CE	LYS E	67	12.938				
	6638	NZ	LYS E	67	13.120	57.655	-11.522	1.00	181.51
65	6639	C	LYS E	67	12.014	64.362	-10.732	1.00	125.36
	6640	0	LYS E	67	12.671	64.622	<i>-</i> 11.737	1.00	125.36
	6641	Ň	CYS E	68	12.289	64.881	-9.541	1.00	114.74
	6642	ĊA	CYS E	68	13.451	65.729	-9.370	1.00	114.74
			CYS E	68	14.297	65.211	-8.210	1.00	114.74
70	6643	C				64.428	-7.388	1.00	114.74
70	6644	0	CYS E	68	13.824	04.440	-7.300	1.00	1 14./4

6846 S.G. CYS E. 68 12.001 67.607 7.729 1.000 167.12		6645	СВ	CYS E	68	13,047	67,197	-9.159	1.00	167.12
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6701 CB GLU E 75 14.992 60.694 -7.316 1.00 206.72 6702 CG GLU E 75 15.456 59.259 -7.100 1.00 206.72 6703 CD GLU E 75 15.456 59.259 -7.100 1.00 206.72 6703 CD GLU E 75 15.605 59.096 -9.159 1.00 206.72 6705 OE2 GLU E 75 15.254 57.465 -8.660 1.00 206.72 6706 C GLU E 75 13.420 61.414 -5.488 1.00 220.79 6707 O GLU E 75 13.071 60.495 -4.747 1.00 220.79 6708 N SER E 76 12.604 62.385 -5.885 1.00 123.65 6710 CB SER E 76 11.211 62.502 -5.457 1.00 123.65 6711 OG SER E 76 10.648 63.837 -5.918 1.00 156.05 6712 C SER E 76 10.583 63.854 -7.332 1.00 156.05 6712 C SER E 76 10.310 61.422 -5.997 1.00 123.65 6713 O SER E 76 10.623 60.793 -7.006 1.00 123.65	22									
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65 6709 CA SER E 76 11.211 62.502 -5.457 1.00 123.65 6710 CB SER E 76 10.646 63.837 -5.918 1.00 156.05 6711 OG SER E 76 10.583 63.854 -7.332 1.00 156.05 6712 C SER E 76 10.310 61.422 -5.997 1.00 123.65 6713 O SER E 76 10.623 60.793 -7.006 1.00 123.65						13.071				
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6713 O SER E 76 10.623 60.793 -7.006 1.00 123.65										
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	6715	CA	GLU E	77	8.193	60.247	-5.762	1.00	207.04
	6716	CB	GLU E	77	7.055	60.135	-4.744	1.00	207.91 181.88
	6717	CG	GLU E	77	7.495	59.613	-3.388	1.00	181.88
_	6718	CD .	GLU E	77	8.000	58.181	-3.440	1.00	181.88
5	6719	OE1	GLU E	77	8.281	57.684	-4.551	1.00	181.88
	6720	OE2	GLU E	77	8.127	57.550	-2.369	1.00	181.88
	6721 6722	C	GLU E GLU E	77 77	7.645 7.050	70. 711 61. 78 8	-7.103 -7.189	1.00 1.00	207.91
	6723	N	PRO E	77 78	7.857	59.919	-7.169 -8.171	1.00	207.91
10	6724	CD	PRO E	78	8.716	58.718	-8.203	1.00	80.79 240.65
	6725	CA	PRO E	78	7.390	60.237	-9.522	1.00	80.79
	6726	СВ	PRO E	78	7.588	58.930	-10.260	1.00	240.65
	6727	ÇG	PRO E	78	8.884	58.468	-9. 399	1.00	240.65
15	6728	C	PRO E	78 70	5.967	60.738	-9 594	1.00	80.79
15	6729 6720	O N	PRO E VAL E	78 79	5.145 5.681	60.436 61.517	-8.738 -10.622	1.00	80.79
	6730 6731	ČA	VAL E	79	4.351	62.067	-10.822	1.00 1.00	112.90 112.90
	6732	CB	VAL E	79	4.314	63.550	-10.455	1.00	137.47
	6733	CG1	VAL E	79	3.032	14.176	-10.987	1.00	137.47
20	6734	CG2	VAL E	79	4.403	63.715	-8.951	1.00	137.47
	6735	C	VAL E	79	3.978	61.908	-12.251	1.00	112.90
	6736	0	VAL E	79	4.737	62.312	-13.132	1.00	112.90
	6737 6738	N CA	TYR E TYR E	80 80	2.807 2.402	61.334 61.134	-12.508 -13.886	1.00 1.00	70.76 70.76
25	6739	CB	TYR E	80	1.630	59.841	-14.062	1.00	159.99
	6740	CG	TYR E	80	1.595	59.441	-15.510	1.00	159.99
	6741	CD1	TYR E	80	2.763	59.078	-16.169	1.00	159.99
	6742	CE1	TYR E	80	2.758	58.714	-17.498	1.00	159.99
30	6743	CD2	TYR E	80	0.408	59.437	-16.231	1.00	159.99
30	6744 6745	CE2 CZ	TYR E TYR E	80 80	0.395 1.583	59.076 58.712	-17.589 -18.206	1.00 1.00	159.99
	6746	OH	TYR E	80	1.597	58.323	-19.528	1.00	159.99 159.99
	6747	Č.	TYR E	80	1.562	62.238	-14.446	1.00	70.76
	6748	Ō	TYR E	80	0.661	62.746	-13.795	1.00	70.76
35	6749	N	LEU E	81	1.838	62.587	-15.684	1.00	117.40
	6750	CA	LEU E	81	1.086	63.620	-16.343	1.00	117.40
	6751	CB CG	LEU E	81	2.037 1.348	64.731 65.705	-16.752	1.00	104.60
	6752 6753	CD1	LEU E	81 81	0.269	65.795 66.455	-17.590 -16.750	1.00 1.00	104.60 104.60
40	6754	CD2	LEU E	81	2.357	66.811	-18.058	1.00	104.60
. •	6755	C	LEU E	81	0.455	62.990	-17.575	1.00	117.40
	6756	0	LEU E	81	1.148	62.313	-18.325	1.00	117.40
	6757	N	GLU E	82	-0.844	63.186	-17.792	1.00	85.04
45	6758 6750	CA CB	GLU E	82	-1.474	62.609	-18.982	1.00	85.04
45	6759 6760	CG	GLU E	82 82	-2.520 -2.736	61.566 60.525	-18.598 -19.684	1.00 1.00	152.39 152.39
	6761	CD	GLU E	82	-3.765	59.482	-19.297	1.00	152.39
	6762	OE1	GLU E	82	-3.785	59.083	-18.107	1.00	152.39
~~	6763	OE2	GLU E	82	-4.542	59.055	-20.185	1.00	152.39
50	6764	Ç	GLU E	82	-2.112	63.691	-19.854	1.00	85.04
	6765	0 N	GLU E VAL E	82 83	-2.843	64.562	-19.363	1.00	85.04
	6766 6767		VAL E	83	-1.829 -2.355	63.634 64.628	-21.152 -22.085	1.00	88.74
	6767 6768	CB CB	VAL E	83	-2.355 -1.258	64.628 65.146	-22.085 -23.010	1.00 1.00	88.74 170.11
55	6769	CG1	VAL E	83	-1.862	66.064	-24.054	1.00	170.11
	6770	CG2	VAL E	83	-0.213	65.878	-22.197	1.00	170.11
	6771	Ç	VAL E	83	-3.482	64.102	-22.949	1.00	88.74
	6772	0	VAL E	83	-3.391	63.013	-23.507	1.00	88.74
60	6773 6774	· N CA	PHE E PHE E	84 84	-4.534 -5.675	64.895 64.451	-23.091 -23.873	1.00 1.00	98.95 98.95
00	6775	CB	PHE E	84	-6.917	64.273	-22.986	1.00	118.45
	6776	õ	PHE E	84	-6.734	63.316	-21.864	1.00	118.45
	6777	CD1	PHE E	84	-5.997	63.674	-20.749	1.00	118.45
<i>(=</i>	6778	CD2	PHE E	84	-7.324	62.065	-21.911	1.00	118.45
65	6779	CE1	PHE E	84	-5.839	62.795	-19.701	1.00	118.45
	6780	CE2 CZ	PHE E	84 94	-7.172 -6.424	61.173	-20.865	1.00	118.45
	6781 6782	c c	PHE E PHE E	84 84	-6.434 -6.114	61.541 65.318	-19.756 -25.034	1.00 1.00	118.45
	6783	ŏ.	PHE E	84	-5.736	66.484	-25.034 -25.178	1.00	、 98.95 98.95
70	6784	N	SER E	85	-6.967	64.697	-25.837	1.00	152.83

	6785	CA	SER E	85	-7.592	65.304	-26.990	1.00	152.83
	6786	CB	SER E	85	-6.937	64.819	-28.279	1.00	197.25
	6787	OG .	SER E	85	-7.565	65.403	-29.405	1.00	197.25
	6788	C .	SER E	85	-9.030	64.791	-26.914	1.00	152.83
5	6789	0	SER E	85	-9.279	63.598	-27.101	1.00	152.83
	6790	N	ASP E	86	-9.962	65.685	-26.600	1.00	101.99
	6791	CA	ASP E	86	-11.375	65.330	-26.494	1.00	101.99
	6792	CB	ASP E	86	-11.573	64.296	-25.386	1.00	136.02
	6793	CG	ASP E	86	-12.655	63.310	-25,715	1.00	136.02
10	6794	OD1	ASP E	86	-13.782	63.752	-26.031	1.00	136.02
	6795	OD2	ASP E	86	-12.375	62.095	-25.664	1.00	136.02
	6796	C	ASP E	86	-12.199	66.594	-26.197	1.00	101.99
	6797	0	ASP E	86	-11.646	67.635	-25.830	1.00	101.99
15	6798	N	TRP E	87	-13.516	66.516	-26.356	1.00	94.76
13	6799	CA	TRP E	87	-14.351	67.689	-26.106	1.00	94.76
	6800 6801	CB CG	TRP E	87	-15.806	67.417	-26.477	1.00	229,11
	6802	CD2	TRP E	87 87	-16.051	67.695	-27.896	1.00	229.11
	6803	CE2	TRP E	87 87	-15.956	66.755	-28.964	1.00	229.11
20	6804	CE3	TRP E	87	-16.120 -15.735	67.470 65.372	-30.165	1.00	229.11
20	6805	CD1	TRP E	87	-16.281	68.917	-29.026 -28.471	1.00	229.11
	6806	NE1	TRP E	87	-16.319	68.787	-29.837	1.00 1.00	229.11
	6807	CZ2	TRP E	87	-16.070	66.850	-31.411	1.00	229.11 229.11
	6808	CZ3	TRP E	87	-15.685	64.755	-30.265	1.00	229.11
25	6809	CH2	TRP E	87	-15.855	65.491	-31.438	1.00	229.11
	6810	С	TRP E	87	-14.273	68.108	-24.671	1.00	94.76
	6811	0	TRP E	87	-13.962	69.260	-24.355	1.00	94.76
	6812	N	LEU E	88	-14.546	67.147	-23.802	1.00	160.64
20	6813	CA	LEU E	88	-14.527	67.385	-22.379	1.00	160.64
30	6814	CB	LEU E	88	-15.912	67.160	-21.803	1.00	93.36
	6815	CG	LEU E	88	-16.950	68.149	-22.276	1.00	93.36
	6816	CD1	LEU E	88	-18.247	67.872	-21.532	1.00	93.36
	6817 6818	CD2	LEU E LEU E	88	-16.456	69.560	-22.001	1.00	93.36
35	6819	C O	LEU E	88 88	-13.553	66.490	-21.645	1.00	160.64
55	6820	Ň	LEU E	89	-13.401 -12.908	65.314 67.057	-21.968	1.00	160.64
	6821	ČA	LEU E	89	-11.961	66.321	-20. 63 5 -19.828	1.00 1.00	107.53
	6822	CB	LEU E	89	-10.552	66.785	-20.131	1.00	107.53 83.31
	6823	CG	LEU E	89	-9.538	66.057	-19.267	1.00	83.31
40	6824	CD1	LEU E	89	-9.821	64.541	-19.311	1.00	83.31
	6825	CD2	LEU E	89	-8.138	66.385	-19.757	1.00	83.31
	6826	Ç	LEV E	89	-12.252	66.573	-18.366	1.00	107.53
	6827	0	LEU E	89	-12.378	67.718	-17.954	1.00	107.53
45	6828	N	LEU E	90	-12.366	65.510	-17.576	1.00	62.89
43	6829 6830	CA CB	LEU E	90	-12.629	65.676	-16.142	1.00	62.89
	6831	CG	LEU E	90	-13.400	64.487	-15.588	1.00	49.26
	6832	CD1	LEU 3	90 90	-13,609 -14,422	64.523 65.760	-14.077	1.00	49.26
	6833	CD2	LEU E	90	-14.422	65.760 63.261	-13.775	1.00	49.26
50	6834	C	LEU E	90	-11.300	65.773	-13.579 -15.404	1.00 1.00	49.26
	6835	ŏ	LEU E	90	-10.515	64.830	-15.410	1.00	62.89 62.89
	6836	Ň	GLN E	91	-11.043	66.907	-14.764	1.00	69.52
	6837	CA	GLN E	91	-9.785	67.083	-14.064	1.00	69.52
	6838	CB	GLN E	91	-9.210	68.449	-14 388	1.00	103.30
55	6839	CG	GLN E	91	-8.977	68.644	-15.857	1.00	103.30
	6840	CD	GLN J	91	-8.226	69.921	-16.149	1.00	103.30
	6841	OE1	GLN E	91	-8.750	71.021	-15.967	1.00	103.30
	6842	NE2	GLN E	91	-6.979	69.783	-16.599	1.00	103.30
60	6843	. C	GLN E	91	-9.965	66.953	-12.584	1.00	69.52
oo	6844	O N	GLN E	91	-10.984	67.372	-12.033	1.00	69.52
	6845 6846	N CA	ALA E	92	-8.972	66.375	-11.925	1.00	61.94
	6847	CB	ALA E ALA E	92	-9.070 9.241	66.223	-10.483	1.00	61.94
	6848	C	ALA E	92 92	-9.241 -7.838	64.773 66.792	-10.125	1.00	129.56
65	6849	ŏ	ALA E	92	-7.636 -6.715	66.663	-9.794 -10.314	1.00 1.00	61.94
-	6850	Ň	SER E	93	-8.045	67.437	-10.314 -8.643	1.00	61.94 82.97
	6851	CA	SER E	93	-6.930	68.004	-7.904	1.00	82.97
	6852	CB	SER E	93	-7.388	68.550	-6.552	1.00	72.43
70	6853	OG.	SER E	93	-8.203	67.620	-5.871	1.00	72.43
70	6854	С	SER E	93	-5.965	66.855	-7.717	1.00	82.97
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	6855	0 N	SER E ALA E	93	-4.873	66.846	-8.282	1.00	82.97
	6856 6857	CA	ALA E ALA E	94 94	-6.395 -5.588	65.865 64.680	-6.948	1.00	109.69
	6858	CB ·	ALA E	94	-5.086	64.711	-6.683 -5.262	1.00 1.00	109.69
5	6859	С	ALA E	94	-6.468	63.455	-6.910	1.00	145.34 109.69
	6860	0	ALA E	94	-7.652	63.488	-6.620	1.00	109.69
	6861	N	GLU E	95	-5.902	62.372	-7.431	1.00	77.50
	6862 6863	CA CB	GLU E	95 95	-6.688 -6.065	61.172	-7.711	1.00	77.50
10	6864	CG	GLU E	95	-5.979	60.391 61.195	-8.859 -10.136	1.00 1.00	137.79
٠,	6865	CD	GLU E	95	-5.700	60.335	-11.358	1.00	137.79 137.79
	6866	OE1	GLU E	95	-5.582	60.901	-12.468	1.00	137.79
	6867	OE2	GLU E	95	-5.607	59.094	-11.210	1.00	137.79
15	6868 6869	C O	GLU E	95 05	-6.869	60.258	-6.514	1.00	77.50
13	6870	N	GLU E VAL E	95 96	-7.723 -6.067	59.376 60.468	-6.538 5.470	1.00	77.50
	6871	ČA	VAL E	96	-6.148	59.673	-5.470 -4.241	1.00 1.00	83.99
	6872	СВ	VAL E	96	-5.042	58. 64 1	-4.191	1.00	83.99 76.64
20	6873	CG1	VAL E	96	-5.384	57.579	-3.164	1.00	76.64
20	6874	CG2	VAL E	96	-4.856	58.037	-5.568	1.00	76.64
	6875 6876	C	VAL E VAL E	96	-6.009	60.634	-3.071	1.00	83.99
	6877	N	VAL E	96 97	-5.127 -6.863	61.491 60.475	-3.057	1.00	83.99
	6878	ĊA	VAL E	97	-6.880	61.409	-2.071 -0.959	1.00 1.00	86.29
25	6879	CB	VAL E	97	-8.028	62.389	-1.152	1.00	86.29 80.14
	6880	CG1	VAL E	97	-7.861	63.550	-0.242	1.00	80.14
	6881	CG2	VAL E	97	-8.102	62.821	-2.571	1.00	80.14
	6882 6883	C O	VAL E	97	-7.073	60.838	0.440	1.00	86.29
30	6884	N	VAL E MET E	97 98	-7.940 -6.305	59.988 61.349	0.646	1.00	86.29
	6885	ĈA	MET E	98	-6.430	60.922	1.405 2.799	1.00 1.00	72.65 72.65
	6886	СВ	MET E	98	-5.268	61.476	3.603	1.00	162.98
	6887	CG	MET E	98	-3.950	60.925	3.147	1.00	162.98
35	6888 6889	SD	MET E	98	-3.643	59.309	3.816	1.00	162.98
22	6890	CE C	MET E	98 98	-3.249 -7.747	59.757 61.457	5.511	1.00	162.98
	6891	ŏ	MET E	98	-7.747 -8.065	62.625	3.359 3.165	1.00 1.00	72.65
	6892	N	GLU E	99	-8.515	60.612	4.042	1.00	72.65 91.21
40	6893	CA	GLU E	99	-9.789	61.038	4.815	1.00	91.21
40	6894	CB	GLU E	99	-10.288	60.011	5.630	1.00	221.21
	6895 6896	CD	GLU E	99 99	-11.780	60.081	5.888	1.00	221.21
	6897	OE1	GLU E	99	-12.193 -11.617	59.288 58.201	7.112 7.342	1.00 1.00	221.21
	6898	OE2	GLU E	99	-13.102	59.747	7.836	1.00	221.21 221.21
45	6899	Ç	GLU E	99	-9.575	62.376	5.322	1.00	91.21
	6900	0	GLU E	99	-8.664	62.499	6.140	1.00	91.21
	6901 6902	N CA	GLY E GLY E	100 100	-10.388 -10.248	63.379	4.993	1.00	149.52
	6903	č	GLY E	100	-9.666	64.679 65.799	5.632 4.782	1.00 1.00	149.52
50	6904	Ō	GLY E	100	-9.830	66.974	5.111	1.00	149.52 149.52
	6905	N	GLN E	101	-8.982	65.450	3.697	1.00	88.18
	6906	CA	GLN E	101	-8.381	66.447	2.803	1.00	88.18
	6907 6908	CB CG	GLN E GLN E	101	-7.183 6.052	65.843	2.072	1.00	168.37
55	6909	CD	GLN E	101 101	-6.053 -5.680	65.456 66.573	2.988 - 3.934	1.00	168.37
	6910	OE1	GLN E	101	-6.363	66.812	4.923	1.00 1.00	168.37 168.37
	6911	NE2	GLN E	101	-4.598	67.272	3.630	1.00	168.37
	6912	C	GLN E	101	-9.334	67.070	1.767	1.00	88.18
60	6913 6914	0 N	GLN E	101	-10.447	66.597	1.540	1.00	88.18
00	6915	CD	PRO E PRO E	102 102	-8.894 -7.628	68.148 68.898	1.116	1.00	90.47
	6916	GA	PRO E	102	-7.026 -9.766	68.772	1.252 0.125	1.00 1.00	130.24 90.47
	6917	CB	PRO E	102	-9.195	70.179	0.022	1.00	130.24
65	6918	çG	PRO E	102	-7.727	69.923	0.124	1.00	130.24
O)	6919 6920	C O	PRO E	102	-9.708	68.020	-1.203	1.00	90.47
	6921	N	PRO E LEU E	102 103	-8.713 -10.775	67.360 68.133	-1.510	1.00	90.47
	6922	CA	LEU E	103	-10.775	67.475	-1.988 -3.283	1.00 1.00	92.93 92.93
70	6923	CB	LEV E	103	-11.638	66.186	-3.160	1.00	78.05
70	6924	CG	LEV E	103	-11.718	65.529	-4.528	1.00	78.05

	6925	CD1	LEU E	103	-10.330	65.172	-4.969	1.00	70.05
	6926	CD2	LEU E	103	-12.618	64.299	-4.466	1.00	78.05 78.05
	6927	Ç	LEU E	103	-11.556	68.364	-4.296	1.00	92.93
5	6928	0	LEU E	103	-12.690	68.784	-4.071	1.00	92.93
3	6929 6930	N	PHE E	104	-10.906	68.654	-5.413	1.00	62.11
	6931	CA CB	PHE E PHE E	104	-11.557	69.491	-6.406	1.00	62.11
	6932	CG	PHE E	104 104	-10.792	70.814	-6.607	1.00	152.14
	6933	CD1	PHE E	104	-10.639 -9.688	71.636 71.298	-5.354	1.00	152.14
10	6934	CD2	PHE E	104	-11.439	71.256	-4.401 5.120	1.00	152.14
	6935	CE1	PHE E	104	-9.537	72.054	-5.132 -3.235	1.00	152.14
	6936	CE2	PHE E	104	-11.297	73.526	-3.967	1.00 1.00	152.14
	6937	CZ	PHE E	104	-10.338	73.173	-3.020	1.00	152.14 152.14
٠.	6938	С	PHE E	104	-11.672	68.775	-7.759	1.00	62.11
15	6939	0	PHE E	104	-10.686	68.246	-8.269	1.00	62.11
	6940	N	LEU E	105	-12.871	68.748	-8.336	1.00	83.91
	6941	CA	LEU E	105	-13.074	68.140	-9.651	1.00	83.91
	6942 6943	CB CG	LEU E	105	-14.208	67.119	-9.618	1.00	47.95
20	6944	CD1	LEU E	105	-14.010	66.057	-8.551	1.00	47.95
	6945	CD2	LEU E	105 105	-15.076 -12.633	64.958	-8.677	1.00	47.95
	6946	Č	LEU E	105	-13.454	65.508 69.279	-8.729	1.00	47.95
	6947	ō	LEU E	105	-14.110	70.224	-10.565 -10.133	1.00	83.91
	6948	Ν .	ARG E	106	-13.063	69.201	-11.824	1.00 1.00	83.91
25	6949	CA	ARG E	106	-13.391	70.273	-12.737	1.00	105.55 105.55
	6950	СВ	ARG E	106	-12.132	71.181	-12.874	1.00	149.26
	6951	CG	ARG E	106	-12.358	72.290	-13.865	1.00	149.26
	6952	CD	ARG E	106	-11.036	72.987	-14.126	1.00	149.26
30	6953 6954	NE OZ	ARG E	106	-11.165	74.010	-15.158	1.00	149.26
30	6955	CZ NH1	ARG E	106	-10.153	74.477	-15.880	1.00	149.26
	6956	NH2	ARG E ARG E	106	-8.925	74.013	-15.691	1.00	149.26
	6957	C	ARG E	106 106	-10.374 -13.804	75.404 60.764	-16.800	1.00	149.26
	6958	ŏ	ARG E	106	-13.044	69.761 69.027	-14.110 -14.734	1.00	105.55
35	6959	N	CYS E	107	-15.000	70.118	-14.585	1.00 1.00	105.55
	6960	CA	CYS E	107	-15.400	69.665	-15.913	1.00	115.02 115.02
	6961	С	CYS E	107	-14.789	70.673	-16.856	1.00	115.02
	6962	O	CYS E	107	-15.230	71.813	-16.932	1.00	115.02
40	6963	CB	CYS E	107	-16.914	69.630	-16.079	1.00	134.10
40	6964 6965	SG N	CYS E	107	-17.441	68.605	-17.498	1.00	134.10
	6966	CA	HIS E HIS E	108	-13.755	70.242	-17.562	1.00	96.54
	6967	CB	HIS E	108 108	-13.017 -11.535	71.109 70.876	-18.460	1.00	96.54
	6968	CG	HIS E	108	-10.657	70.876 71.846	-18.240 -18.959	1.00	124.72
45	6969	CD2	HIS E	108	-9.644	71.651	-19.836	1.00 1.00	124.72
	6970	ND1	HIS E	108	-10.737	73.207	-18.759	1.00	124.72 124.72
	6971	CE1	HIS E	108	-9.806	73.807	-19.480	1.00	124.72
	6972	NE2	HIS E	108	-9.128	72.886	-20.142	1.00	124.72
50	6973	Ç	HIS E	108	-13. 328	70.954	-19.938	1.00	96.54
50	6974 6975	0	HIS E	108	-13.224	69.864	-20.506	1.00	98.54
	6976	N CA	GLY E GLY E	109	-13.680	72.070	-20.563	1.00	176.91
	6977	C	GLY E	109 109	-13.999	72.050	-21.973	1.00	177.91
	6978	ŏ	GLY E	109	-12.753 -11.727	72.194 72.706	-22.815	1.00	176.91
55	6979	Ň	TRP E	110	-11.737 -12.826	72.706 71.732	-22.349	1.00	176.91
	6980	CA	TRP E	110	-11.696	71.836	-24.056 -24.956	1.00	146.96
	6981	CB	TRP E	110	-11.982	71.061	-26.241	1.00 1.00	146.96 177.84
	6982	CG	TRP E	110	-10.936	71,248	-27.286	1.00	177.84
60	6983	CD2	TRP E	110	-9.797	70.415	-27.514	1.00	177.84
60	6984	CE2	TRP E	110	-9.056	70.996	-28.564	1.00	177.84
	6985	CE3	TRP E	110	-9.331	69.226	-26.932	1.00	177.84
	6986	CD1	TRP E	110	-10.845	72.273	-28.180	1.00	177.84
	6987 6988	NE1	TRP E	110	-9.718	72.131	-28.953	1.00	177.84
65	6989	CZ2 CZ3	TRP E TRP E	110	-7.875	70.433	-29.047	1.00	177.84
33	6990	CH2	TRP E	110	-8.153	68.667	·27.413	1.00	177.84
	6991	C	TRP E	110 110	-7.439 -11.404	69.273 73.303	-28.459	1.00	177.84
	6992	ŏ	TRP E	110	-11.404	73.303 74.154	-25.275 -25.255	1.00	146.96
	6993	Ň	ARG E	111	-10.136	74.154 73.594	-25.255 -25.551	1.00	146.96
70	6994	CA	ARG E	111	-9.716	74.948	-25.887	1.00 1.00	199.97
				-	•		-0.007	1.00	199.97

	6995	CB	ARG E	111	-10.136	75.282	-27.295	1.00	249.42
	6996	CG	ARG E	111	-9.116	74.871	-28.285	1.00	249.42
	6997	CD.	ARG E	111	-9.462	75.454	-29.595	1.00	249.42
5	6998	NE .	ARG E	111	-8.270	75.956	-30.249	1.00	249.42
J	6999 7000	CZ NH1	ARG E	111	-7.559	76.996	-29.814	1.00	249.42
	7000	NH2	ARG E ARG E	111	-7.918	77.656	-28.711	1.00	249.42
	7002	C	ARG E	111 111	-6.472	77.367	-30.483	1.00	249.42
	7003	ŏ	ARG E	111	-10.262 -10.388	76.009	-24.972	1.00	199.97
10	7004	Ň	ASN E	112	-10.597	77.173 75.590	-25.350	1.00	199.97
_	7005	CA	ASN E	112	-11.129	76.482	-23.767 -22.769	1.00	112.19
	7006	CB	ASN E	112	-10.101	77.553	-22.432	1.00	112.19
	7007	CG	ASN E	112	-10.330	78.144	-21.061	1.00 1.00	133.79
	7008	OD1	ASN E	112	-11.446	78.097	-20.531	1.00	133.79 133.79
15	7009	ND2	ASN E	112	-9.280	78.710	-20.478	1.00	133.79
	7010	Č	ASN E	112	-12.445	77.147	-23.163	1.00	112.19
	7011	0	ASN E	112	-12.776	78.218	-22.651	1.00	112.19
	7012	N	TRP E	113	-13.200	76.532	-24.067	1.00	154.00
20	7013	CA	TRP E	113	-14.478	77.116	-24.441	1.00	154.00
20	7014 7015	CB CG	TRP E	113	-15.153	76.326	-25.542	1.00	235.27
	7016	CD2	TRP E	113	-14.586	76.595	-26.860	1.00	235.27
	7017	CE2	TRP E	113	-14.400	75.651	-27.909	1.00	235.27
	7018	CE3	TRP E	113 113	-13.885	76.353	-29.018	1.00	235.27
25	7019	CD1	TRP E	113	-14.628 -14.180	74.270	-28.027	1.00	235.27
	7020	NE1	TRP E	113	-13.758	77.804 77.667	-27.348	1.00	235.27
	7021	CZ2	TRP E	113	-13.592	75.726	-28.647 -30.229	1.00	235.27
	7022	CZ3	TRP E	113	-14.335	73.643	-30.229 -29. 23 3	1.00	235.27
	7023	CH2	TRP E	113	-13.818	74.373	-30.318	1.00 1.00	235.27
30	7024	С	TRP E	113	-15.400	77.133	-23.246	1.00	235.27 154.00
	7025	0	TRP E	113	-14.983	76.886	-22.116	1.00	154.00
	7026	N	ASP E	114	-16.664	77.430	-23.503	1.00	242.58
	7027	CA	ASP E	114	-17.649	77.470	-22,442	1.00	242.58
35	7028 7029	CB	ASP E	114	-18.418	78.794	-22.471	1.00	249.32
25	7030	CG OD1	ASP E ASP E	114	-17.656	79.922	-21.803	1.00	249.32
	7030	OD2	ASP E	114	-17.348	79.791	-20.599	1.00	249.32
	7032	C	ASP E	114 114	-17.365 -18.606	80.933	-22.475	1.00	249.32
	7033	ŏ	ASP E	114	-19.027	76.306 75.942	-22.572	1.00	242.58
40	7034	N	VAL E	115	-18.931	75.717	-23.672 -21.430	1.00	242.58
	7035	CA	VAL E	115	-19.846	74,594	-21.391	1.00 1.00	148.92
	7036	CB	VAL E	115	-19.199	73.377	-20.746	1.00	148.92 243.92
	7037	CG1	VAL E	115	-20.086	72.162	-20.949	1.00	243.92
15	7038	CG2	VAL E	115	-17.821	73.161	-21.331	1.00	243.92
45	7039	C	VAL E	115	-21.075	74.959	-20.581	1.00	148.92
•	7040	0	VAL E	115	-20.985	75.672	-19.577	1.00	148.92
	7041 7042	N CA	TYR E	116	-22.226	74.466	-21. 0 20	1.00	86.50
	7042	CB	TYR E TYR E	116	-23.470	74.752	-20.320	1.00	86.50
50	7044	CG	TYRE	116 116	-24.374	75.633	-21.192	1.00	249.77
-	7045	CD1	TYR E	116	23.782 -23.088	76.991 .	-21.517	1.00	249.77
	7046	CE1	TYR E	116	-23.066 -22.513	77.210 78.454	-22.709	1.00	249.77
	7047	CD2	TYR E	116	-23.889	78.048	-22.994 -20.616	1.00	249.77
	7048	CE2	TYR E	116	-23.319	79.293	-20.886	1.00	249.77
55	7049	CZ	TYR E	116	-22.631	79.488	•22. 07 5	1.00 1.00	249.77
	7050	OH	TYR E	116	-22.051	80.710	-22.336	1.00	249.77 249.77
	7051	С	TYR E	116	-24.208	73.466	-19.940	1.00	86.50
	7052	0	TYR E	116	-23.829	72.356	-20.362	1.00	86.50
60	7053	N.	LYS E	117	-25.277	73.630	-19.164	1.00	217.77
00	7054	CA	LYS E	117	-26.078	72.500	-18.707	1.00	217.77
	7055	CB	LYS E	117	-26.963	71.967	-19.832	1.00	191.92
	7056 7057	CG	LYS E	117	-28.295	72.674	-19.997	1.00	191.92
	7057 7058	CE	LYS E	117	-29.246	71.813	-20.819	1.00	191.92
65	7059	NZ	LYS E Lys e	117 117	-29.481	70.462	-20.143	1.00	191.92
	7060	C	LYS E	117	-30.376 -25.161	69.560	-20.915	1.00	191.92
	7061	ŏ	LYS E	117	-25.228	71.387 70.262	-18.230	1.00	217.77
	7062	Ň	VAL E	118	-24.306	70.262 71.709	-18.724 -17.269	1.00	217.77
	7063	CA	VAL E	118	-23.356	70.743	-17.268 -16.731	1.00	181.28
70	7064	CB	VAL E	118	-22.089	71.444	-16.254	1.00 1.00	181.28
		•						1.00	157.61

	7065	CG1	VAL E	118	-21.427	70.628	-15.171	1.00	157.61
	7066	ÇG2	VAL E	118	-21.141	71.619	-17.420	1.00	157.61
	7067 7068	C .	VAL E	118	-23.857	69.864	-15.598	1.00	181.28
5	7069	Ŋ	VAL E	118	-24.500	70.335	-14.661	1.00	181.28
	7070	ČA	ILE E	119 119	-23.514 -23.932	68.585	-15.674	1.00	95.37
	7071	CB	ILE E	119	-25.932 -25.093	67.630 66.783	-14.665	1.00	95.37
	7072	CG2	ILE E	119	-25.598	65.858	-15.184 -14.102	1.00	80.86
	7073	CG1	ILE E	119	-26.198	67.695	-15.696	1.00 1.00	80.86
10	7074	CD1	ILE E	119	-27.227	66.956	-16.527	1.00	80.86 80.86
	7075	Ç	ILE E	119	-22.791	66.678	-14.348	1.00	95.37
	7076	0	ILE E	119	-22.280	66.017	-15.249	1.00	95.37
	7077 7078	N	TYR E	120	-22.373	66.602	13.088	1.00	103.71
15	7079	CA CB	TYR E TYR E	120	-21.315	65.664	-12.732	1.00	103.71
	7080	CG	TYR E	120 120	-20.499 -19.634	66.128	11.550	1.00	87.63
	7081	CD1	TYR E	120	-20.141	67.303 68.575	-11.821	1.00	87.63
	7082	CE1	TYR E	120	-19.351	69.666	-11.746 -12.010	1.00	87.63
••	7083	CD2	TYR E	120	-18.300	67.141	-12.171	1.00 1.00	87.63
20	7084	CE2	TYR E	120	-17.486	68.226	-12.447	1.00	87.63
	7085	CZ	TYR E	120	-18.017	69.490	-12.366	1.00	87.63 87.63
	7086	он	TYR E	120	-17.220	70.579	-12.651	1.00	87.63
	7087 7088	C	TYR E	120	-21.972	64.380	-12.305	1.00	103.71
25	7089	N	TYR E TYR E	120	-23.037	24.401	-11.694	1.00	103.71
20	7090	CA	TYR E	121 121	-21.324	63.263	-12.596	1.00	62.69
	7091	CB	TYR E	121	-21.857 -22.202	61.963 61.148	-12.221	1.00	62.69
	7092	CG	TYR E	121	-23.364	61.653	-13.476 -14.309	1.00	95.66
-	7093	CD1	TYR E	121	-23.288	62.865	-14.992	1.00 1.00	95.66
30	7094	CE1	TYR E	121	-24.334	63.305	-15.806	1.00	95.66 95.66
	7095	CD2	TYR E	121	-24.522	60.885	-14.455	1.00	95.66
	7096 7097	CE2	TYR E	- 121	-25.576	61.315	-15.269	1.00	95.66
	7097	CZ OH	TYR E TYR E	121	-25.477	62.527	-15. 94 5	1.00	95.66
35	7099	C C	TYR E TYR E	121 121	-26.515 -20.873	62.943	-16.761	1.00	95.66
	7100	ŏ	TYR E	121	-20.673 -19.667	61.165 61.179	-11.368	1.00	62.69
	7101	N	LYS E	122	-21.391	60.478	-11.620 -10.356	1.00	62.69
	7102	CA	LYS E	122	-20.562	59.633	-9.521	1.00 1.00	76.05 76.05
40	7103	CB	LYS E	122	-20.410	60.198	-8.114	1.00	107.43
40	7104	CG	LYS E	122	-19.516	59.339	-7.238	1.00	107.43
	7105 7106	CD CE	LYS E	122	-19.635	59.698	-5.779	1.00	107.43
	7107	NZ	LYS E Lys e	122	-18.887	58.706	-4.914	1.00	107.43
	7108	C	LYS E	122 122	-19.161 -21.223	58.998 58.263	-3.484	1.00	107.43
45	7109	ŏ	LYS E	122	-22.325	58.127	-9.440 -8.898	1.00	76.05
	7110	N	ASP E	123	-20.543	57.252	-9.973	1.00 1.00	76.05
	7111	CA	ASP E	123	-21.059	55.892	-9.976	1.00	138.97 138.97
	7112	CB	ASP E	123	-21.188	55.363	-8.545	1.00	185.30
50	7113	CG	ASP E	123	-19.849	54.991	-7.945	1.00	185.30
50	7114 7115	OD1 OD2	ASP E ASP E	123	-19.068	54.303	-8.638	1.00	185.30
	7116	C	ASP E	123 123	-19.578	55.374 55.374	-6.785	1.00	185.30
	7117	ŏ	ASP E	123	-22.396 -23.333	55.792 55.147	-10.702	1.00	138.97
	7118	N	GLY E	124	-22.472	56.443	-10.225 -11.862	1.00	138.97
55	7119	CA	GLY E	124	-23.675	56.412	-12.675	1.00 1.00	163.35
	7120	C	GLY E	124	-24.838	57.262	-12.200	1.00	163.35 163.35
	7121	0	GLY E	124	-25.840	57.388	-12.907	1.00	163.35
	7122 7123	N	GLU E	125	-24.711	57.854	-11.016	1.00	131.17
60	7123	CA CB	GLU E GLU E	125	-25.777	58.684	-10.447	1.00	131.17
•	7125	CG	GLU E	125 125	-25.822	58.535	-8.911	1.00	143.41
	7126	CD	GLU E	125	-26.269 -27.780	57.168 56.071	-8.368	1.00	143.41
	7127	OE1	GLU E	125	-28.492	56.971 57.744	-8.384 -7.700	1.00	143.41
	7128	OE2	GLU E	125	-28.249	56.040	-7.700 -9.077	1.00	143.41
65	7129	Ç	GLU E	125	-25.597	60.160	-10.771	1.00 1.00	143.41 131.17
	7130	0	GLU E	125	-24.483	60.656	-10.809	1.00	131.17
	7131	N CA	ALA E	126	-26.695	60.864	-11.006	1.00	115.32
	7132 7133	CA CB	ALA E	126	-26.604	62.290	-11.265	1.00	115.32
70	7134	CB	ALA E ALA E	126	-27.979	62.844	-11.605	1.00	168.61
		J	VPV E	126	-26.104	62.855	-9.935	1.00	115.32
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	7135	0	A1 A F	400	00.40	****			
	7136	0 N	ALA E LEU E	126	-26.467	62.339	-8.876	1.00	115.32
	7137	CA		127	-25.275	63.897	-9.967	1.00	118.41
	7137	CB .	LEU E	127	-24.752	64.458	-8.714	1.00	118.41
5	7139	CG	LEU E	127 127	-23.271 -22.934	64.162	-8.577	1.00	111.80
-	7140	CD1	LEU E	127	·22.834 ·23.811	64.190 63.158	-7.090	1.00	111.80
	7141	CD2	LEU E	127	-23.611	63.889	-6.384	1.00	111.80
	7142	C	LEU E	127	-24.957	65.947	-6.868	1.00	111.80
	7143	ŏ	LEU E	127	-25.470	66.328	-8.453 -7.404	1.00	118.41
10	7144	Ň	LYS E	128	-24.498	66.785	-7.404 -9.373	1.00	118,41
	7145	CA	LYS E	128	-24.677	68.228	-9.259	1.00	133.41
	7146	СВ	LYS E	128	-23.405	68.893	-8.760	1.00	133.41
	7147	CG	LYS E	128	-22.965	68.445	-7.388	1.00	171.72
	7148	CD	LYS E	128	-23.865	68.977	-7.388 -6.284	1.00	171.72
15	7149	CE	LYS E	128	-23.287	68.616	-0.264 -4.917	1.00	171.72
	7150	NZ	LYS E	128	-24.024	69.227	-3.779	1.00	171.72
	7151	C	LYS E	128	-25.015	68.757	-10.653	1.00	171.72
	7152	Ö	LYS E	128	-24.626	68.153	-11.657	1.00 1.00	133.41
	7153	N	TYR E	129	-25.733	69.87	-10.729		133.41
20	7154	CA	TYR E	129	-26.106	70.442	-12.029	1.00 1.00	159.58
	7155	CB	TYR E	129	-27.496	69.983	-12.438	1.00	159.58
	7156	CG	TYR E	129	-28.122	70.887	-13.441	1.00	246.12
	7157	CD1	TYR E	129	-27.756	70.809	-14.781	1.00	246.12
	7158	CE1	TYR E	129	-28.298	71.675	-15.715	1.00	246.12
25	7159	CD2	TYR E	129	-29.063	71.857	-13.055	1.00	246.12
	7160	CE2	TYR E	129	-29.624	72.721	-13.990	1.00	246.12
	7161	CZ	TYR E	129	-29.236	72.624	-15.326	1.00	246.12 246.12
	7162	OH	TYR E	129	-29.822	73.442	-16.274	1.00	246.12
•	7163	С	TYR E	129	-26.106	71.953 .	-12.048	1.00	159.58
30	7164	0	TYR E	129	-26.579	72.589	-11.112	1.00	159.58
	7165	N	TRP E	130	-25.600	72,526	-13.137	1.00	184.49
	7166	CA	TRP E	130	-25.557	73.976	-13.280	1.00	184.49
	7167	CB	TRP E	130	-24.211	74.535	-12.817	1.00	245.42
25	7168	CG	TRP E	130	-23.751	74.067	-11.472	1.00	245.42
35	7169	CD2	TRP E	130	-23.750	74.828	-10.257	1.00	245.42
	7170	CE2	TRP E	130	-23.186	74.005	-9.254	1.00	245.42
	7171	CE3	TRP E	130	-24.179	76.119	-9.918	1.00	245.42
	7172	CD1	TRP E	130	-23.202	72.856	-11.1 6 6	1.00	245.42
40	7173	NE1	TRP E	130	-22.859	72.811	-9.835	1.00	245.42
40	7174	CZ2	TRP E	130	-23.034	74.438	-7.930	1.00	245.42
	7175 7176	CZ3	TRP E	130	-24.028	76.548	-8.600	1.00	245.42
	7177	CH2	TRP E	130	-23.454	75.709	-7.626	1.00	245.42
	7178	C	TRPE	130	-25.768	74.407	-14.725	1.00	184.49
45	7179	O N	TRPE	130	-25.711	73.584	-15.638	1.00	184.49
1.5	7180	CA	TYR E TYR E	131	-26.014	75.701	-14.930	1.00	185.41
	7181	CB	TYRE	131 131	-26.187	76.228	-16 <i>.</i> 277	1.00	185.41
	7182	ČĠ	TYRE	131	-27.063 -27.438	77.477	-16.282	1.00	249.42
	7183	CD1	TYR E	131	-27.436 -28.391	77.858 77.406	-17.685	1.00	249.42
50	7184	CE1	TYR E	131	-28.654	77.125	-18.389	1.00	249.42
	7185	CD2	TYP E	131	-26.755	77.384 78.869	-19.728	1.00	249.42
	7186	CE2	TYR E	131	-26.997	79.127	-18.358	1.00	249.42
	7187	CZ	TYR E	131	-27.951	78.384	-19.703	1.00	249.42
	7188	ОH	TYR E	131	-28.189	78.642	-20.380	1.00	249.42
55	7189	Ċ	TYR E	131	-24.780	76.577	-21.710 -16.758	1.00	249.42
	7190	Ō	TYTE	131	-24.141	75.784	-10.756 -17.455	1.00	185.41
	7191	N	GLU E	132	-24.310	77.777	-16.415	1.00	185.41
	7192	CA	GLU E	132	-22.942	78.159	-16.751	1.00 1.00	229.70
	7193	CB	GLU E	132	-22.638	79.608	-16.344	1.00	229.70
60	7194	CG	GLU E	132	-23.207	80.700	-17.258	1.00	249.20
	7195	CD	GLU E	132	-22.123	81.565	-17.898	1.00	249.20
	7196	OE1	GLU E	132	-20.982	81.562	-17.392	1.00	249.20
	7197	OE2	GLU E	132	-22.412	82.255	-18.899	1.00	249.20
/-	7198	C	GLU E	132	-22.290	77.200	-15.773	1.00	249.20 229.70
65	7199	0	GLU E	132	-22.652	77.190	-14.595	1.00	
	7200	N	ASN E	133	-21.348	76.385	-16.233	1.00	229.70 219.94
	7201	CA	ASN E	133	-20.764	75.401	-15.332	1.00	219.94
	7202	CB	ASN E	133	-19.878	74.415	-16.095	1.00	129.08
70	7203	CG	ASN E	133	-18.469	74.898	-16.252	1.00	129.08
70	7204	OD1	ASN E	133	-18.235	76.020	-16.692	1.00	129.08
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	7205	ND2	ASN E	133	-17.510	74.046	-15.904	1.00	100.00
	7206	С	ASN E	133	-20.023	75.919	-14.118	1.00	129.08
	7207	Ó	ASN E	133	-19.802	77.115	-13.944		219.94
	7208	Ñ.	HIS E	134	-19.638			1.00	219.94
5	7209	CA	HIS E			74.965	-13.286	1.00	192.14
,	7210	CB		134	-18.970	75.231	-12.036	1.00	192.14
			HIS E	134	-20.007	75.079	-10.924	1.00	214.14
	7211	CG	HIS E	134	-19.514	75.463	-9.567	1.00	214.14
	7212	CD2	HIS E	134	-19.356	74.731	-8.436	1.00	214.14
• •	7213	ND1	HIS E	134	-19.138	76.749	-9.245	1.00	214.14
10	7214	CE1	HIS E	134	-18.771	76.794	-7.976	1.00	
	7215	NE2	HIS E	134	-18.895	75.584	-7.463		214.14
	7216	С	HIS E	134	-17.828	74.231		1.00	214.14
	7217	ŏ	HIS E				-11.860	1.00	192.14
	7218	Ñ		134	-17.412	73.574	-12.820	1.00	192.14
15			ASN E	135	-17.336	74.114	-10.630	1.00	109.49
13	7219	CA	ASN E	135	-16.246	73.208	-10.311	1.00	109.49
	7220	CB	ASN E	135	-14.921	73.967	-10.346	1.00	216.32
	7221	CG	ASN E	135	-14.571	74.433	-11.741	1.00	216.32
	7222	OD1	ASN E	135	-14.694	73.661	-12.691	1.00	
	7223	ND2	ASN E	135	-14.125	75.677	-11.883		216.32
20	7224	C	ASN E	135	-16.462			1.00	216.32
	7225	ŏ	ASN E			72.573	-8.957	1.00	109.49
	7226	Ň		135	-15.960	73.058	-7.948	1.00	109.49
			ILE E	136	-17.223	71.484	-8.949	1.00	98.56
	7227	, CA	ILE E		-17.541	70.753	·7.725	1.00	98.56
25	7228	C8	ILE E	136	-18.026	69.322	8.063 - پ	1.00	164.42
25	7229	CG2	ILE E	136	-17.070	68.654	-9.020	1.00	164.42
	7230	CG1	ILE E	136	-18.182	68.505	-6.792	1.00	
	7231	CD1	ILE E	136	-18.771	67.146			164.42
	7232	Č	ILE E	136			-7.055	1.00	164.42
	7233	ŏ	ILE E		-16.351	70.717	-6.779	1.00	98.56
30	7234	Ň		136	-15.300	70.168	-7.104	1.00	98.56
50			SER E	137	-16.524	71.329	-5.613	1.00	114.80
	7235	CA	SER E	137	-15.462	71.405	-4.622	1.00	114.80
	7236	СВ	SER E	137	-15.128	72.866	-4.360	1.00	96.11
	7237	OG	SER E	137	-14.336	72.997	-3.196	1.00	96.11
	7238	С	SER E	137	-15.798	70.714	-3.303	1.00	
35	7239	0	SER E	137	-16.955	70.690	-2.879		114.80
	7240	N	ILE E	138	-14.773	70.169		1.00	114.80
	7241	CA	ILE E	138			-2.652	1.00	105.32
	7242	CB	ILE E		-14.939	69.466	-1.382	1.00	105.32
	7243	CG2		138	-14.851	67.969	-1.577	1.00	81.88
40			ILE E	138	-14.767	67.296	-0.223	1.00	81.88
TV	7244	CG1	ILE E	138	-16.049	67.484	-2.408	1.00	81.88
	7245	CD1	ILE E	138	-15.917	66.048	-2.912	1.00	81.88
	7246	С	ILE E	138	-13.869	69.833	-0.374	1.00	105.32
	7247	0	ILE E	138	-12.686	69.614	-0.619	1.00	105.32
	7248	N	THR E	139	-14.283	70.362	0.772	1.00	128.39
45	7249	CA	THR E	139	-13.333	70.758	1.807	1.00	
	7250	СВ	THR E	139	-13.986	71.743			128.39
	7251	OG1	THR E	139			2.788	1.00	173.54
	7252	CG2	THR E		-15.220	71.194	3.265	1.00	173.94
	7253			139	-14.267	73.071	2.094	1.00	173.94
50		Ç	THR E	139	-12.825	69.535	2.566	1.00	128.39
20	7254	0	THR E	139	-11.709	69.058	2.337	1.00	128.39
	7255	N	ASN E	140	-13.650	69.041	3.480	1.00	224.25
	7256	CA	ASN E	140	-13.323	67.859	4.263	1.00	224.25
	7257	CB	ASN E	140	-14.012	67.918	5.625		
	7258	CG	ASN E	140	-13.813	66.656		1.00	231.48
55	7239	OD1	ASN E	140			6.429	1.00	231.48
	7260	ND2	ASN E		-13.998	65.547	5.923	1.00	231.43
	7261			140	-13.443	66.823	7.692	1.00	231.40
		C	ASN E	140	-13.874	66.691	3.464	1.00	224.25
	7262	0	ASN E	140	-15.073	66.629	3.204	1.00	224.25
60	7263	N	ALÁ E	141	-13.004	65.763	3.086	1.00	132.13
60	7264	CA	ALA E	141	-13.420	64.623	2.289	1.00	132.13
	7265	CB	ALA E	141	-12.374	64.323	1.257		
	7266	C	ALA E	141	-13.730	63.367		1.00	95.25
	7267	ŏ	ALA E	141			3.072	1.00	132.13
	7268	Ň			-12.932	62.901	3.884	1.00	132.13
65	7269		THR E	142	-14.903	62.811	2.802	1.00	103.70
05		CA	THR E	142	-15.339	61.588	3.454	1.00	103.70
	7270	CB	THR E	142	-16.873	61.526	3.477	1.00	152.79
	7271	OG1	THR E	142	-17.384	62.747	4.028	1.00	152.79
	7272	CG2	THR E	142	-17.346	60.376	4.329	1.00	152.79
=-	7273	С	THR E	142	-14.767	60.417	2.650		
70	7274	0	THR E	142	-14.198	60.624		1.00	103.70
			-	- ·-		00.0E7	1.575	1.00	103.70

	7275	N	VAL E	143	-14.887	59.197	3.164	1.00	124.54
	7276	CA	VAL E	143	-14.369	58.042	2.437	1.00	124.54
	7277	CB.	VAL E	143	-14.026	56.863	3.365	1.00	132.81
5	7278	CG1	VAL E	143	-15.292	56.315	3.999	1.00	132.81
٦	7279	CG2	VAL E	143	-13.310	55.773	2.577	1.00	132.81
	7280	C	VAL E	143	-15.448	57.583	1.484	1.00	124.54
	7281	0	VAL E	143	-15.187	56.822	0.555	1.00	124.54
	7282	N	GLU E	144	-16.668	58.047	1.722	1.00	123.03
10	7283	CA	GLU E	144	-17.781	57.678	0.863	1.00	123.03
10	7284 7285	CB CG	GLU E	144	-19.108	57.964	1.558	1.00	249.45
		CD	GLU E	144	-19.323	57.136	2.812	1.00	249.45
	7286 7287	OE1	GLU E GLU E	144	-19.316	57.978	4.073	1.00	249.45
	7288	OE2		144	-20.163	58.892	4.176	1.00	249.45
15	7289	C	GLU E	144	-18.470	57.730	4.958	1.00	249.45
13	7299 7290	Ö	GLU E GLU E	144	-17.709	58.428	-0.460	1.00	123.03
	7290 7291	N	ASP E	144	-18.373	58.051	-1.416	1.00	123.03
	7292	CA	ASP E	145	-16.897	59.485	-0.509	1.00	78.25
	7293	CB	ASP E	145	-16.721	60.284	-1.726	1.00	78.25
20	7294	CG	ASP E	145 145	-16.017	61.593	-1.396	1.00	126.03
20	7295	OD1	ASP E	145	-16.912 -17.955	62.551 62.900	-0.679	1.00	126.03
	7296	OD2	ASP E	145			-1.272	1.00	126.03
	7297	C	ASP E	145	-16.581	62.944	0.465	1.00	126.03
	7298	ŏ	ASP E	145	-15.918 -15.889	59.528	-2.789	1.00	78.25
25	7299	Ň	SER E	146	-15.263	59.920	-3.952	1.00	78.25
	7300	CA	SER E	146	-14.482	58.442 57.660	-2.388	1.00	91.78
	7301	CB	SER E	146	-13.708	56.568	-3.331	1.00	91.78
	7302	OG OG	SER E	146	-12.805	57.145	-2.591	1.00	200.20
	7303	Č	SER E	146	-15.448	57.145 57.065	-1.661 4.335	1.00	200.20
30	7304	ŏ	SER E	146	-16.558	56.675	-4.335 -3.981	1.00	91.78
	7305	Ň	GLY E	147	-15.039	57.020	-5.592	1.00 1.00	91.78
	7306	CA	GLY E	147	-15.910	56.484	-6.622	1.00	97.94
	7307	C	GLY E	147	-15.365	56.777	-8.007	1.00	97.94 97.94
	7308	ŏ	GLY E	147	-14.177	57.079	-8.146	1.00	97.94 97.94
35	7309	Ň	THR E	148	-16.211	56.677	-9.033	1.00	66.84
	7310	CA	THR E	148	-15.767	56.955	-10.399	1.00	66.84
	7311	CB	THR E	148	-15.794	55.674	-11.285	1.00	76.59
	7312	OG1	THR E	148	-16.932	55.699	-12.141	1.00	76.59
	7313	CG2	THR E	148	-15.880	54.450	-10.424	1.00	76.59
40	7314	С	THR E	148	-16.662	58.055	-10.978	1.00	66.84
	73 15	0	THR E	148	-17.884	57.889	-11.145	1.00	66.84
	7316	N	TYR E	149	-16.041	59.187	-11.273	1.00	55.84
	7317	CA	TYR E	149	-16.768	60.335	-11.774	1.00	55.84
4.5	7318	CB	TYR E	149	-16.262	61.585	-11.070	1.00	63.87
45	7319	CG	TYR E	149	-16.445	61.611	-9 .575	1.00	63.87
	7320	CD1	TYR E	149	-15.728	60.766	-8.730	1.00	63.87
	7321	CE1	TYR E	149	-15.895	60.837	-7.34 2	1.00	63.87
	7322	CD2	TYR E	149	-17.326	62.515	-9.003	1.00	63.87
50	7323	CE2	TYR E	149	-17.502	62.597	-7.63 9	1.00	63.87
30	7324	CZ	TYR E	149	-16.793	61.761	-6.812	1.00	63.87
	7325	ОН	TYR E	149	-17.022	61.871	-5.455	1.00	63.87
	7326	C	TYR E	149	-16.630	60.541	-13.274	1.00	55.84
	7327	O.	TYR E	149	-15.789	59.909	-13.918	1.00	55.84
55	7328	N OA	TYR E	150	-17.478	61.414	-13.817	1.00	90.25
23	7329	CA	TYR E	150	-17.463	61.805	-15.227	1.00	90.25
	7330	CB	TYR E	150	-17.811	60.622	-16.175	1.00	141.76
	7331 7332	CG	TYR E	150	-19.266	60.196	-16.334	1.00	141.76
		CD1	TYR E	150	-20.183	60.995	-17.006	1.00	141.76
60	7333 7334	CE1	TYR E	150	-21.503	60.584	-17.180	1.00	141.76
UU	7335	CD2	TYR E	150	-19.711	58.965	-15.839	1.00	141.76
	7336	CE2	TYR E	150	-21.030	58.545	-16.010	1.00	141.76
	7336 7337	CZ OH	TYR E	150	-21.924	59.359	-16.678	1.00	141.76
	7337 7338		TYR E	150	-23.239	58.958	-16.823	1.00	141.76
65	7339	C	TYR E TYR E	150	-18.481	62.934	-15.293	1.00	90.25
55	7340	Ň	CYS E	150 151	-19.308	63.056	-14.388	1.00	90.25
	7341	ČA.	CYS E	151	-18.404 -19.360	63.792	-16.309	1.00	89.54
	7342	č	CYS E	151	-19.945	64.895 65.031	-16.421	1.00	89.54
	7343	ŏ	CYS E	151	-19.354	65.031 64.573	-17.811	1.00	89.54
70	7344	ČВ	CYS E	151	-18.713	64.573 66.218	-18.778 -16.017	1.00	89.54
			J.J L	.51	10.713	00.210	-16.017	1.00	116.04

	7345	SG	CYS E	151	-17.189	66.664	-16.901	1.00	116.04
	7346	N	THR E	152	-21.118	65.650	-17.904	1.00	
	7347	CA	THR E		-21.783	65.851	-19.186	1.00	145.06
	7348	CB ·	THR E		-23.138	65.100	-19.247		145.06
5	7349	OG1	THR E		-24.059	65.683		1.00	246.19
•	7350	CG2	THR E				-18.316	1.00	246.19
	7351		THR E		-22.944	63.634	-18.897	1.00	246.19
		C			-22.032	67.345	-19.332	1.00	145.06
	7352	0	THR E		-22.255	68.039	-18.337	1.00	145.06
10	7353	N	GLY E	153	-21.984	67.845	-20.562	1.00	193.40
10	7354	CA	GLY E		-22.209	69.263	-20.777	1.00	193.40
	7355	С	GLY E	153	-22.478	69.578	-22.227	1.00	193.40
	7356	0	GLY E	153	-22.181	68.768	-23.105	1.00	
	7357	N	LYS E	154	-23.044	70.751	-22.486	1.00	193.40
	7358	CA	LYS E	154	-23.331	71.135	-23.857		120.13
15	7359	CB	LYS E	154				1.00	120.13
••	7360	CG			-24.722	71.763	-23.950	1.00	168.61
			LYS E		-25.193	72.073	-25.366	1.00	168.61
	7361	CD	LYS E	154	-26.607	72.634	-25.316	1.00	168.61
	7362	CE	LYS E		-27.120	73.053	-26.682	1.00	168.61
00	7363	NZ	LYS E	154	-28.455	73.682	-26.542	1.00	168.61
20	7364	С	LYS E	154	-22.271	72.122	-24.309	1.00	120.13
	7365	0	LYS E	154	-21.969	73.090	-23.596	1.00	120.13
	7366	N	VAL E	155	-21.685	71.856	-25.475	1.00	
	7367	CA	VAL E	155	-20.666	72.731			169.05
	7368	CB	VAL E	155			-26.041	1.00	169.05
25	7369	CG1			-19.362	71.985	-26.310	1.00	148.26
45				155	-18.328	72.927	-26.910	1.00	148.26
	7370	CG2	VAL E	` 155	-18.847	71.420	-25.025	1.00	148.26
	7371	C	VAL E	155	-21.235	73.223	-27.351	1.00	169.05
	7372	0	VAL E	155	-21.684	72.425	-28.174	1.00	169.05
	7373	N	TRP E	156	-21.207	74.537	-27.537	1.00	249.39
30	7374	CA	TRP E	156	-21.767	75.132	-28.733	1.00	
	7375	СВ	TRP E	156	-21.199	74.494	-29.991		249.39
	7376	CG	TRP E	156	-19.797			1.00	249.75
	7377	CD2	TRP E			74.775	-30.144	1.00	249.75
	7378	CE2	TOO	156	-19.204	76.069	-30.193	1.00	249.75
35			TRP E	156	-17.813	75.880	-30.292	1.00	249.75
55	7379	CE3	TRP E	156	-19.720	77.368	-30.164	1.00	249.75
	7380	CD1	TRP E	156	-18.784	73.875	-30.220	1.00	249.75
	7381	NE1	TRP E	156	-17.583	74.533	-30.307	1.00	249.75
	7382	CZ2	TRP E	156	-16.919	76.947	-30.375	1.00	249.75
	7383	CZ3	TRP E	156	-18.838	78.426	-30.229	1.00	249.75
40	7384	CH2	TRP E	156	-17.440	78.210	-30.344	1.00	
	7385	C	TRP E	156	-23.225	74.814			249.75
	7386	Õ	TRP E	156	-24.004		-28.688	1.00	249.39
	7387	Ň	GLN E			75.512	-28.053	1.00	249.39
	7388	ČA		157	-23.571	73.711	-29.338	1.00	249.35
45	7389		GLN E	157	-24.945	73.299	-29.404	1.00	249.35
73		CB	GLN E	157	-25.559	73.927	-30.645	1.00	249.42
	7390	cc	GLN E	157	-25.723	75.415	-30.458	1.00	249.42
	7391	CD	GLN E	157	-26.491	75.691	-29.186	1.00	249,42
	7392	OE1	GLN E	157	-27.538	75.108	-28.977	1.00	249.42
	7393	NE2	GLN E	157	-25.980	76.575	-28.340	1.00	
50	7394	С	GLN E	1	-25.152	71.797	-29.367	1.00	249.42
	7395	0	GLN E	157	-26.238	71.302			249.35
	7396	Ň	LEU E	158	-24.109		-29.670	1.00	249.35
	7397	ČA	LEU E			71.074	-28.973	1.00	232.10
	7398		LEU E	158	-24.192	69.626	-28.872	1.00	232.10
55		CB		158	-23.321	68.956	-29.935	1.00	212.17
<i>J</i> J	7399	CG	LEU E	158	-23.853	68.895	-31.367	1.00	212.17
	7400	CD1	LEU E	158	-23.486	67.531	-31.928	1.00	212.17
	7401	CD2	LEU E	158	-25.370	69.079	-31.415	1.00	212.17
	7402	С	LEU E	158	-23.788	69.124	-27.492	1.00	232.10
	7403	0	LEU E	158	-23.007	69.767	-26.784		
60	7404	N	ASP E	159	-24.333			1.00	232.10
	7405	ČA	ASP E	159		67.969 67.353	-27.122	1.00	245.44
	7406	CB	ASP E		-24.058	67.353	-25.830	1.00	245.44
	7407		400 E	159	-25.270	66.525	-25.381	1.00	211.53
		CG	ASP E	159	-26.567	67.329	-25.373	1.00	211.53
65	7408	OD1	ASP E	159	-26.659	68.326	-24.626	1.00	211.53
65	7409	OD2	ASP E	159	-27.502	66.961	-26.118	1.00	211.53
	7410	С	ASP E	159	-22.822	66.454	-25.908	1.00	245.44
	7411	0	ASP E	159	-22.578	65.818	-26.936		
	7412	Ň	TYR E	160	-22.046	66.411	-26.836 -24.824	1.00	245.44
								1.00	160 E/
		CA		160					168.54
70	7413 7414	CA CB	TYR E	160 160	-20.842 -19.592	65.579 66.368	-24.759 -25.140	1.00	168.54 216.78

74107 CEI TYR E 180 -20.188 88.381 -26.533 1.00 216.78 7419 CEI TYR E 160 -20.270 89.041 -27.747 1.00 216.78 7419 CEZ TYR E 160 -19.081 89.096 -27.644 1.00 216.78 7419 CEZ TYR E 160 -19.081 89.097 -28.688 1.00 216.78 7421 CH TYR E 150 -20.003 89.045 -28.0414 1.00 216.78 7422 CH TYR E 160 -20.003 89.045 -28.0414 1.00 216.78 7422 CH TYR E 160 -20.003 89.045 -28.0414 1.00 168.54 7423 O TYR E 160 -20.003 89.045 -28.0414 1.00 168.54 7424 N GUU E 161 -19.738 83.004 -22.2351 1.00 168.54 7425 CA GUU E 161 -19.738 83.004 -22.2351 1.00 168.54 7426 CB GUU E 161 -19.738 83.004 -22.200 1.00 174.81 7427 CG GUU E 161 -20.076 89.447 -22.330 1.00 174.81 7428 CB GUU E 161 -20.076 89.447 -22.330 1.00 174.81 7429 OE1 GUU E 161 -20.765 89.447 -20.632 1.00 174.81 7429 OE1 GUU E 161 -20.765 89.447 -20.632 1.00 174.81 7430 OE2 GUU E 161 -20.765 89.447 -20.632 1.00 174.81 7430 OE2 GUU E 161 -20.765 89.447 -20.632 1.00 174.81 7431 OE2 GUU E 161 -20.765 89.447 -20.632 1.00 174.81 7432 O C GUU E 161 -20.688 99.686 -21.241 1.00 174.81 7433 O C GUU E 161 -20.688 99.686 -21.241 1.00 174.81 7435 CA SER E 162 -16.648 63.065 -20.067 1.00 118.65 7433 O C GUU E 161 -17.223 82.6689 -20.067 1.00 118.65 7435 CB SER E 162 -16.648 63.065 -20.067 1.00 118.65 7435 CB SER E 162 -16.648 63.065 -20.067 1.00 118.65 7437 C SER E 162 -16.648 63.065 -20.067 1.00 118.65 7438 O G SER E 162 -16.648 63.065 -20.067 1.00 118.65 7438 O SER E 162 -16.648 63.065 -20.067 1.00 118.65 7439 N GUU E 163 -14.275 89.972 -20.073 1.00 118.65 7436 CB SER E 162 -16.548 63.065 -20.067 1.00 118.65 7437 C SER E 162 -15.548 63.065 -18.315 1.00 104.28 7444 O C G GUU E 163 -14.478 63.065 -18.315 1.00 104.28 7445 C C G GUU E 163 -14.478 63.065 -18.315 1.00 104.28 7446 C C G GUU E 163 -14.778 61.391 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.		7415	CG	TYR E	160	-19.684	67.078	-26.461	1.00	216.78
7418 CD2 TYR E 160 -19.001 66.446 -27.644 1.00 24.675 7420 CZ TYR E 160 -19.001 67.097 -28.686 1.00 216.76 7421 OH TYR E 160 -20.003 69.045 -28.686 1.00 216.77 7422 C TYR E 160 -20.003 69.045 -28.686 1.00 216.78 7423 O TYR E 160 -20.003 69.045 -20.001 10.00 168.54 7424 N GLU E 161 -20.048 53.771 -23.399 1.00 118.65 7425 CA GLU E 161 -20.048 53.771 -23.399 1.00 118.65 7426 CA GLU E 161 -20.048 53.771 -23.399 1.00 118.65 7427 CG GLU E 161 -20.0778 61.624 -22.300 1.00 174.81 7428 CG GLU E 161 -20.078 61.624 -22.300 1.00 174.81 15 7429 CG GLU E 161 -20.078 58.446 -21.241 1.00 174.81 15 7429 CG GLU E 161 -20.078 58.446 -21.241 1.00 174.81 7431 C G GLU E 161 -20.078 58.446 -21.225 1.00 174.81 7431 C G GLU E 161 -20.078 58.446 -21.2267 1.00 174.81 7433 N SER E 162 -17.688 63.066 -21.0267 1.00 174.81 7433 N SER E 162 -17.688 63.066 -20.0877 1.00 174.81 7435 CG SER E 162 -16.584 63.055 -20.0877 1.00 174.81 7436 CG SER E 162 -16.584 63.055 -20.0877 1.00 118.65 7437 C SER E 162 -16.584 63.055 -20.0877 1.00 118.65 7438 O G SER E 162 -16.584 63.055 -20.0877 1.00 118.65 7439 O G SER E 162 -16.589 63.005 -20.0877 1.00 118.65 7439 O G SER E 162 -16.589 63.005 -20.0877 1.00 118.65 7439 O G SER E 162 -16.589 63.005 -20.0877 1.00 118.65 7439 O G SER E 162 -16.589 63.005 -20.0877 1.00 118.65 7439 O G SER E 162 -16.589 60.0725 -20.057 1.00 111.30 7440 C G GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7441 C G GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7444 O G GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7444 O G GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7446 C G GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7447 O GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7446 C G GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7447 O GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7448 N PRO E 164 -14.478 61.391 -20.272 1.00 64.59 7489 CD PRO E 164 -14.584 57.008 1.1865 1.00 64.59 7485 CG RO E 164 -14.584 57.008 1.1866 1.00 64.59 7486 C G ANN E 166 -11.590 57.407 -14.554 1.00 64.59 7487 C G GLU E 163 -14.478 61.391 -20.272 1.00 64.59 7487 C G G GLU E 165		7416 7417	CD1	TYR E	160	-20.168	68.381	-26.533	1.00	216.78
5 7419 CE2 TYR E 160 -19.807 63.935 -28.969 1.00 12.07 7420 CZ TYR E 160 -20.036 89.045 -28.969 1.00 216.73 7421 OH TYR E 160 -20.059 64.973 -23.333 1.00 168.54 7422 C TYR E 160 -20.059 64.973 -23.333 1.00 168.54 7422 C TYR E 160 -20.069 64.973 -23.333 1.00 168.54 7422 C TYR E 160 -20.089 65.561 -22.351 1.00 168.54 7422 C TYR E 160 -20.089 65.561 -22.351 1.00 168.54 7422 C TYR E 161 -20.048 63.771 -23.399 1.00 118.65 7426 C R GLU E 161 -20.048 63.771 -23.399 1.00 118.65 7426 C R GLU E 161 -20.078 61.624 -22.303 1.00 174.81 7427 C G GLU E 161 -20.076 60.665 -21.205 1.00 174.81 7427 C G GLU E 161 -20.107 60.665 -21.205 1.00 174.81 7428 C D GLU E 161 -20.765 58.447 -20.632 1.00 174.81 7430 C C GLU E 161 -20.765 58.447 -20.632 1.100 174.81 7430 C G GLU E 161 -20.765 58.447 -20.632 1.100 174.81 7430 C G GLU E 161 -18.214 62.850 -22.067 1.00 174.81 7430 C G GLU E 161 -18.214 62.850 -22.067 1.00 174.81 7432 C G GLU E 161 -18.214 62.850 -22.067 1.00 174.81 7432 C G GLU E 161 -18.214 62.850 -22.067 1.00 174.81 7435 C G G GLU E 161 -18.214 62.850 -20.675 1.00 174.81 7435 C G G GLU E 161 -18.214 62.850 -20.675 1.00 174.81 7436 C G GLU E 161 -18.214 62.850 -20.675 1.00 174.81 7436 C G GLU E 163 -14.76 80 GLO E 20.675 1.00 174.81 7436 C G GLU E 163 -14.478 61.351 2.00 1.00 111.13 7436 C G GLU E 163 -14.478 61.351 2.00 1.00 111.13 7441 C G GLU E 163 -14.478 61.351 2.00 1.00 111.13 7441 C G GLU E 163 -14.478 61.351 2.00 1.00 111.13 7441 C G GLU E 163 -12.417 60.050 -20.257 1.00 111.11 1.00 240.41 7445 C G GLU E 163 -12.417 60.050 -20.257 1.00 111.11 1.00 240.41 7445 C G GLU E 163 -13.515 58.527 2.20.30 1.00 240.41 7445 C G GLU E 163 -14.478 61.351 58.527 2.20.30 1.00 240.41 7445 C G GLU E 163 -12.077 58.972 2.21.731 1.00 240.41 7445 C G GLU E 163 -12.077 58.972 2.21.731 1.00 240.41 7445 C G GLU E 163 -12.077 58.972 2.21.731 1.00 240.41 7445 C G GLU E 163 -12.077 58.972 2.21.731 1.00 240.41 7445 C G GLU E 163 -12.077 58.972 2.21.731 1.00 240.41 7445 C G GLU E 165 -10.047 58.955 59.599 1.22.738 1.00 63.52 7460 C G GLU E 165 -10										
7420 CZ TYR E 150 -19.887 88.395 -28.900 1.00 216.78 7421 7422 CC TYR E 150 -20.003 89.045 -30.114 1.00 216.78 7422 CC TYR E 150 -20.003 89.045 -30.114 1.00 216.78 7423 CC TYR E 150 -20.088 8.973 -23.383 1.00 188.85 7427 7428 CR GLU E 161 -20.048 83.771 -23.399 1.00 188.85 7427 7425 CR GLU E 161 -20.048 83.771 -23.399 1.00 188.85 7427 7426 CB GLU E 161 -20.578 61.624 -22.300 1.00 174.81 7426 CD GLU E 161 -20.578 59.466 -21.205 1.00 174.81 7427 CG GLU E 161 -20.578 59.466 -21.205 1.00 174.81 7429 CD GLU E 161 -20.7785 59.447 -20.652 1.00 174.81 7430 CD GLU E 161 -20.7785 59.447 -20.652 1.00 174.81 7431 C GLU E 161 -20.7785 59.439 -21.241 1.00 174.81 7431 C GLU E 161 -17.529 62.655 -21.205 1.00 174.81 7431 C GLU E 161 -17.529 62.655 -23.085 1.00 174.81 7432 CO GLU E 161 -17.529 62.655 -23.085 1.00 174.81 7432 CO GLU E 161 -18.214 62.890 -22.067 1.00 174.81 7432 CO GLU E 161 -18.214 62.890 -20.067 1.00 174.81 7435 CR SER E 162 -116.249 63.005 -20.643 1.00 174.81 7435 CR SER E 162 -116.249 63.005 -20.643 1.00 171.13 7435 CR SER E 162 -116.249 63.005 -20.643 1.00 171.13 7435 CR SER E 162 -15.464 63.955 1.9512 1.00 104.26 7437 C SER E 162 -15.464 63.955 1.9512 1.00 104.26 7437 C SER E 162 -15.464 63.955 1.9512 1.00 104.26 7437 C SER E 162 -15.464 63.955 1.9512 1.00 104.26 7437 C G GLU E 163 1.4577 61.391 -20.272 1.00 89.90 7444 C G G GLU E 163 1.4578 61.391 1.00 104.26 7447 C G GLU E 163 1.4578 61.391 1.00 104.26 7447 C G GLU E 163 1.4578 61.391 1.00 104.26 7449 C G G GLU E 163 1.4578 61.391 1.00 104.26 7449 C G G GLU E 163 1.4578 61.391 1.00 104.26 7449 C G G GLU E 163 1.4578 61.391 1.90 1.9441 1.00 64.59 7448 C G G GLU E 163 1.4578 61.391 1.90 1.9441 1.00 64.59 7448 C G G GLU E 163 1.4578 61.391 1.90 1.9441 1.00 64.59 7448 C G G GLU E 163 1.4578 61.391 1.90 1.9491 1.00 64.59 7449 C G G GLU E 163 1.4588 61.00 67.00 1.9586 1.00 67.49 7449 C G G GLU E 163 1.4588 61.00 67.00 1.9586 1.00 67.49 7445 C G G GLU E 163 1.4588 61.00 67.00 1.9586 1.00 67.49 7445 C G G GLU E 163 1.4588 61.00 67.00 1.9586 1.00 67.49 7445 C G G G	5									216.78
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15 7429 OE1		7428	CD	GLU E						
7430	15			GLU E	161					
7432				GLU E	161	-22.138			1.00	
7432 O GLU E 161 -17.529 62.655 23.085 1.00 118.65 7433 N SER E 162 -16.749 63.066 -20.877 1.00 111.13 7435 C8 SER E 162 -16.849 63.005 20.643 1.00 111.13 7435 C8 SER E 162 -16.548 63.055 1.95.12 1.00 104.26 7437 C SER E 162 -16.548 63.955 1.95.12 1.00 104.26 7437 C SER E 162 -16.548 63.816 1.83.15 1.00 104.26 7437 C SER E 162 -16.549 63.055 20.057 1.00 111.13 25 7438 O SER E 162 -16.590 60.725 20.057 1.00 111.13 26 7440 CA GLU E 163 -14.478 61.391 20.272 1.00 88.90 7440 CA GLU E 163 -12.917 60.050 20.253 1.00 240.41 7441 CB G GLU E 163 -12.417 60.050 20.253 1.00 240.41 7442 CG GLU E 163 -12.572 58.00 20.253 1.00 240.41 7443 OE1 GLU E 163 -12.359 58.606 22.321 1.00 240.41 7444 OE1 GLU E 163 -12.359 58.606 22.321 1.00 240.41 7446 C GLU E 163 -11.812 57.609 21.802 1.00 240.41 7447 O GLU E 163 -14.478 58.557 23.303 1.00 240.41 7448 N PRO E 164 -14.628 60.795 17.668 1.00 89.90 7448 N PRO E 164 -14.638 60.795 17.668 1.00 89.90 7450 CA PRO E 164 -14.576 57.360 18.645 1.00 64.59 7451 CB PRO E 164 -14.576 57.360 18.686 1.00 66.59 7452 CG PRO E 164 -14.584 55.333 -17.882 1.00 100.06 7453 C PRO E 164 -12.243 58.317 -16.606 1.00 64.59 7455 CG PRO E 164 -12.243 58.317 -16.656 1.00 64.59 7455 CG PRO E 164 -12.243 58.317 -16.656 1.00 64.59 7456 CA PRO E 165 -13.405 58.777 -14.554 1.00 77.47 7457 CB LEU E 165 -13.405 58.777 -14.554 1.00 93.16 7460 CD LEU E 165 -13.405 58.777 -14.554 1.00 93.16 7460 CD LEU E 165 -13.405 58.777 -14.554 1.00 93.16 7460 CD LEU E 165 -13.405 58.777 -14.554 1.00 93.16 7467 CD LEU E 165 -13.405 58.777 -14.554 1.00 93.16 7467 CD LEU E 165 -13.405 58.077 -12.688 1.00 93.16 7467 CD LEU E 165 -13.405 58.077 -12.688 1.00 93.16 7467 CD LEU E 165 -13.405 58.077 -12.688 1.00 93.16 7467 CD LEU E 165 -10.047 60.607 -12.688 1.00 93.16 7467 CD LEU E 165 -10.047 60.607 -12.688 1.00 93.16 7467 CD LEU E 165 -10.047 60.607 -12.688 1.00 93.16 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 93.16 7477 C LEU E 165 -10.047 60.607 -12.688 1.00 93.16 7478 C LEU E 165 -10.047 60.607 -12.688 1.00 93.16 7479 C LEU E 165 -10.0				GLU E		-18.214	62.890			118.65
20 7434 CA SER E 162 -17.688 63.066 -20.877 1.00 111.13 7435 CB SER E 162 -16.249 63.005 -20.643 1.00 111.13 7436 OG SER E 162 -16.648 63.955 -19.512 1.00 104.26 7437 C SER E 162 -16.548 63.955 -19.512 1.00 104.26 7438 O SER E 162 -16.548 63.955 -19.512 1.00 104.26 7438 O SER E 162 -16.548 63.916 -18.315 1.00 104.26 7438 O SER E 162 -16.549 63.616 -18.315 1.00 104.26 7440 CA GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7441 CB GLU E 163 -12.417 60.050 -20.253 1.00 89.90 7441 CB GLU E 163 -12.417 60.050 -20.253 1.00 89.90 7442 CG GLU E 163 -12.417 60.050 -20.253 1.00 240.41 7445 OCI GLU E 163 -12.472 59.972 -21.731 1.00 240.41 7446 CG GLU E 163 -11.812 57.609 -21.802 1.00 240.41 7447 O GLU E 163 -14.131 53.8557 -23.303 1.00 240.41 7447 O GLU E 163 -14.131 53.8557 -23.303 1.00 240.41 7447 O GLU E 163 -14.131 53.8557 -23.303 1.00 240.41 7448 N PRO E 164 -14.028 60.795 -17.668 1.00 89.90 7449 CD PRO E 164 -14.578 57.360 -18.788 1.00 89.90 7451 CB PRO E 164 -14.578 57.360 -18.788 1.00 10.06 7452 CG PRO E 164 -14.578 57.360 -18.078 1.00 64.59 7455 N LEU E 165 -13.224 55.333 -17.682 1.00 10.06 7457 CB PRO E 164 -14.594 55.333 -17.682 1.00 10.06 7457 CB PRO E 164 -14.594 55.333 -17.682 1.00 10.06 7457 CB EU E 165 -13.405 55.333 -17.682 1.00 10.06 7457 CB PRO E 164 -14.594 55.333 -17.682 1.00 10.06 7458 CG LEU E 165 -10.848 61.831 -12.800 1.00 64.59 7458 CG LEU E 165 -10.047 60.607 -12.688 1.00 77.47 7456 CA LEU E 165 -10.088 61.831 -12.800 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.800 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.800 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.207 -12.688 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.800 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.207 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.207 1.00 63.52 7468 CG LEU E 165 -10.088 61.831 -12.207 1.00 63.52 7469 C LEU E 165 -10.088 61.831 -12.207 1.00 63.52 7460 CG LEU E 165 -10.089 57.633 -9.582 1.00 63.52 7460 CG LEU E 165 -10.089 57.633 -9.582 1.00 63.52 7460 CG LEU E 165 -10.089 57.633 -9.582 1.00 63.52 7460					161		62.655	-23.085		
7435 CB SER E 162 -16.249 63.005 -20.643 1.00 104.26 7436 OG SER E 162 -16.848 63.955 -19.512 1.00 104.26 7437 C SER E 162 -16.548 63.955 -19.512 1.00 104.26 7437 C SER E 162 -16.549 63.955 -19.512 1.00 104.26 7438 O SER E 162 -16.609 60.725 -20.057 1.00 111.13 7439 N GLU E 163 -14.478 61.391 -20.272 1.00 89.90 7441 CB GLU E 163 -12.417 60.050 -20.253 1.00 240.41 7442 CG GLU E 163 -12.417 60.050 -20.253 1.00 240.41 7443 CD GLU E 163 -12.272 S9.972 -21.731 1.00 240.41 7444 OE1 GLU E 163 -12.259 58.606 -22.321 1.00 240.41 7445 CC GLU E 163 -12.259 58.606 -22.321 1.00 240.41 7446 C GLU E 163 -13.128 59.527 -23.303 1.00 240.41 7447 OG LU E 163 -13.128 59.527 -23.303 1.00 240.41 7448 N PPO E 164 -14.576 57.360 -18.458 1.00 89.90 7448 N PPO E 164 -14.576 57.360 -18.788 1.00 89.90 7450 CA PRO E 164 -14.576 57.360 -18.788 1.00 69.90 7451 CB PRO E 164 -14.576 57.360 -18.788 1.00 64.59 7452 CG PRO E 164 -14.589 58.395 -16.606 1.00 64.59 7453 C D PRO E 164 -14.589 58.395 -16.606 1.00 64.59 7455 CB PRO E 164 -14.584 57.008 -16.588 1.00 100.06 7457 CB LEU E 165 -12.243 58.317 -16.415 1.00 64.59 7458 CG PRO E 164 -14.584 57.008 -16.588 1.00 100.06 7459 CD PRO E 164 -14.589 59.890 -13.7882 1.00 100.06 7451 CB LEU E 165 -12.243 58.317 -16.415 1.00 64.59 7452 CG PRO E 164 -14.589 59.891 -13.788 1.00 100.06 7453 C C PRO E 164 -15.248 57.008 -16.588 1.00 64.59 7459 CD LEU E 165 -10.047 60.607 -12.688 1.00 64.59 7459 CD LEU E 165 -13.405 58.777 -14.554 1.00 77.47 7457 CB LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 63.52 7460 CD LEU E 165 -10.047 60.607 -12.688 1.00 64.50 7477 C	20					-17.688	63.066	-20.877	1.00	
7436 OG SER E 162 -16.546 63.955 -19.512 1.00 104.26 7437 C SER E 162 -16.548 63.616 -18.315 1.00 104.26 7438 O SER E 162 -15.790 61.603 -20.296 1.00 111.13 7438 O SER E 162 -15.790 61.603 -20.296 1.00 111.13 7440 CA GLU E 163 -14.478 61.391 -20.277 1.00 89.90 7441 CB GLU E 163 -14.478 61.391 -20.277 1.00 89.90 7441 CB GLU E 163 -12.417 60.050 -20.253 1.00 240.41 7442 CG GLU E 163 -12.072 59.972 -21.731 1.00 240.41 7443 CD GLU E 163 -12.072 59.972 -21.731 1.00 240.41 7444 OE1 GLU E 163 -11.812 57.609 -21.802 1.00 240.41 7445 OE2 GLU E 163 -11.812 57.609 -21.802 1.00 240.41 7446 C GLU E 163 -14.131 59.856 18.455 1.00 240.41 7447 O GLU E 163 -14.131 59.856 18.455 1.00 89.90 7448 N PRO E 164 -14.433 58.609 -18.601 1.00 89.90 7449 CD PRO E 164 -14.576 57.360 18.768 1.00 99.90 7451 CB PRO E 164 -14.576 57.360 -18.768 1.00 00.65.59 7452 CG PRO E 164 -14.586 57.360 -18.768 1.00 00.66.59 7453 C PRO E 164 -14.586 57.360 -18.768 1.00 00.66.59 7453 C PRO E 164 -14.586 57.360 -18.768 1.00 00.66.59 7454 O PRO E 164 -14.596 57.360 -18.768 1.00 00.66.59 7455 CA PRO E 164 -14.586 57.360 -18.768 1.00 00.66.59 7456 CA LEU E 165 -13.045 58.377 -14.554 1.00 100.06 7454 O PRO E 164 -12.243 58.317 -16.415 1.00 00.66.59 7455 CB LEU E 165 -13.405 58.777 -14.554 1.00 77.47 7456 CA LEU E 165 -13.405 58.777 -14.554 1.00 77.47 7457 CB LEU E 165 -10.047 60.607 -13.378 1.00 00.77.47 7458 CG LEU E 165 -10.047 60.607 -13.388 1.00 77.47 7459 CD LEU E 165 -10.047 60.607 -13.388 1.00 00.77.47 7450 CD LEU E 165 -10.047 60.607 -13.388 1.00 00.77.47 7451 CB LEU E 165 -10.047 60.607 -13.388 1.00 00.77.47 7452 CA LEU E 165 -10.047 60.607 -13.388 1.00 00.77.47 7453 C G LEU E 165 -10.047 60.607 -13.388 1.00 00.77.47 7456 CA LEU E 165 -13.405 58.709 -13.388 1.00 00.77.47 7457 CB LEU E 165 -10.047 60.607 -13.388 1.00 00.06 63.52 7460 CD2 LEU E 165 -10.047 60.607 -13.388 1.00 00.06 63.52 7461 C C ANN E 166 -11.584 55.601 -10.635 1.00 93.16 7462 C A LEU E 165 -11.771 60.364 -13.329 9.337 1.00 93.16 7468 CB ANN E 166 -11.544 57.651 -10.614 1.00 96.38 7467 C	20			SER E				-20.643	1.00	
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7462 O LEU E 165 -13.328 58.803 -11.665 1.00 77.47 7463 N ASN E 166 -11.580 57.407 -11.959 1.00 93.16 7464 CA ASN E 166 -11.684 56.801 -10.635 1.00 93.16 7465 CB ASN E 166 -11.050 55.421 -10.614 1.00 96.38 7466 CG ASN E 166 -12.037 54.314 -10.900 1.00 96.38 7467 OD1 ASN E 166 -13.220 54.408 -10.581 1.00 96.38 7468 ND2 ASN E 166 -13.220 54.408 -10.581 1.00 96.38 7469 C ASN E 166 -10.999 57.633 -9.582 1.00 93.16 7470 O ASN E 166 -9.975 58.232 -9.837 1.00 93.16 7471 N ILE E 167 -11.544 57.639 -8.380 1.00 64.50 7472 CA ILE E 167 -10.971 58.424 -7.303 1.00 64.50 7473 CB ILE E 167 -11.751 59.709 -7.114 1.00 67.49 7474 CG2 ILE E 167 -11.452 60.314 -5.762 1.00 67.49 7475 CG1 ILE E 167 -11.452 60.314 -5.762 1.00 67.49 7476 CD1 ILE E 167 -11.457 60.672 -8.243 1.00 67.49 7477 C ILE E 167 -12.043 62.011 -8.046 1.00 67.49 7478 O ILE E 167 -12.043 62.011 -8.046 1.00 67.49 7479 N THR E 168 -9.983 57.632 -5.266 1.00 64.50 7480 CA THR E 168 -9.997 56.899 -4.025 1.00 85.23 7481 CB THR E 168 -9.997 55.692 -4.075 1.00 118.46 7483 CG2 THR E 168 -9.470 54.848 -5.162 1.00 118.46										63.52
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100 -9.621 57.759 -2.856 1.00 85.23	70									118.46
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	7485	0	THR E	168	-8.681	58.558	-2.931	4.00	
	7486	N	VAL E	169	-10.379	57.600		1.00	85.23
	7487	CA	VAL E	169	-10.150	58.320	-1.781	1.00	97.28
	7488	CB .	VAL E	169			-0.544	1.00	97.28
5	7489	CG1	VAL E		-11.420	59.087	-0.122	1.00	79.18
-	7490	CG2		169	-11.346	59.434	1.333	1.00	79.18
			VAL E	169	-11.565	60.340	-0.927	1.00	79.18
	7491	Č	VAL E	169	-9.809	57.241	0.489	1.00	97.28
	7492	0	VAL E	169	-10.681	56.475	0.905	1.00	97.28
4.0	7493	N	ILE E	170	-8.538	57.156	0.876	1.00	
10	7494	CA	ILE E	170	-8.113	56.159	1.856		87.96
	7495	СВ	ILE E	170	-6.663	55.682		1.00	87.96
	7496	CG2	ILE E				1.574	1.00	99.84
	7497			170	-6.530	55.259	0.124	1.00	99.84
		CG1	ILE E	170	-5.666	56.808	1.822	1.00	99.84
15	7498	CD1	ILE E	170	-4.217	56.427	1.528	1.00	99.84
15	7499	С	ILE E	170	-8,209	56.759	3.253	1.00	87.96
	7500	0	ILE E	170	-8.544	57.933	3.392	1.00	
	7501	N	LYS E	171	-7.932	55.970			87.96
	7502	CA	LYS E	171	-8.001		4.286	1.00	171.73
	7503	CB	LYS E	171		56.486	5.650	1.00	171.73
20	7504	CG			-9.242	55.^^3	6.353	1.00	217.19
20			LYS E	171	-9.308	54.421	6.380	1.00	217.19
	7505	CD	LYS E	171	-10.739	53.932	6.537	1.00	217.19
	7506	CE	LYS E	171	-11.376	54.437	7.821	1.00	217.19
	7507	NZ	LYS E	171	-12.786	53.971	7.947	1.00	
	7508	С	LYS E	171	-6.749	5o.162	6.454		217.19
25	7509	. 0	LYS E	171	-6.573	56.658		1.00	171.73
	7510	C1	NAG E	221			7.565	1.00	171.73
	7511	C2	NAG E		0.947	78.578	-23.161	1.00	249.29
				221	-0.412	79.265	-23.224	1.00	249.29
	7512	N2	NAG E	221	-1.456	78.261	-23.255	1.00	249.29
20	7513	C7	NAG E	221	-2.671	78.553	-22.807	1.00	249.29
30	7514	07	NAG E	221	-2.963	79.651	-22.339	1.00	
	7515	C8	NAG E	221	-3.720	77.456	-22.880		249.29
	7516	CЗ	NAG E	221	-0.518	80.128		1.00	249.29
	7517	03	NAG E	221	-1.714		-24.473	1.00	249.29
	7518	C4				80.890	-24.425	1.00	249.29
35	7519	O4	NAG E	221	0.670	81.073	-24.631	1.00	249.29
55			NAG E	221	0.579	81.653	-25.947	1.00	249.29
	7520	C5	NAG E	221	1.997	80.296	-24.470	1.00	249.29
	7521 .	O5	NAG E	221	1.994	79.555	-23.228	1.00	249.29
	7522	C6	NAG E	221	3.222	81.198	-24.429	1.00	
	7523	O6	NAG E	221	3.160	82.105	-23.335		249.29
40	7524	C1	NAG E	222	1.316	82.790		1.00	249.29
	7525	C2	NAG E	222			-26.227	1.00	249.77
	7526	N2	NAG E		0.449	83.797	-27.008	1.00	249.77
	7527			222	-0.713	84.171	-26.221	1.00	249.77
		C7	NAG E	222	-0.903	85.441	-25.867	1.00	249.77
45	7528	07	NAG E	222	-0.130	86.350	-26.178	1.00	249.77
43	7529	C8	NAG E	222	-2.140	85.750	-25.043	1.00	249.77
	7530	C3	NAG E	222	0.003	83.194	-28.351	1.00	
	7531	O3	NAG E	222	-0.664	84.182	-29.124		249.77
	7532	C4	N/.G E	· 222	1.211	82.656		1.00	249.77
	7533	04	NAG E	222			-29.133	1.00	249.77
50	7534	C5	NAG E		0.762	81.952	-30.285	1.00	249.77
-	7535	O5		222	2.048	81.716	-28.248	1.00	249.77
			NAG E	222	2.440	82.386	-27.023	1.00	249.77
	7536	C6	NAG E	222	3.319	81.240	-28. 9 26	1.00	249.77
	7537	O6	NAG E	222	3.494	79.843	-28.749	1.00	
	7538	C1	NAG E	242	6.691	58.325	-21.511		249.77
55	7539	C2	NAG E	242	6.772	58.888		1.00	184.18
	7540	N2	IC.S E	242	7.616		-22.927	1.00	184.18
	7541	C7	NAG E	242		60.057	-22.949	1.00	184.18
	7542	07			8.669	60.081	-23.755	1.00	184.18
	7543		NAG E	242	8.972	59.137	-24.489	1.00	184.18
60		C8	NAG E	242	9.523	61.338	-23.746	1.00	184.18
w	7544	C3	NAG E	242	5.382	59.264	-23.429	1.00	184.18
	7545	03	NAG E	242	5.460	59.693	-24.778	1.00	184.18
	7546	C4	NAG E	242	4.452	58.056	-23.332	1.00	
	7547	04	NAG E	242	3.102	58.481			184.18
	7548	CS	NAG E	242			-23.616	1.00	184.18
65	7549	O5			4.513	57.446	-21.911	1.00	184.18
55	7550		NAG E	242	5.874	57.166	-21.520	1.00	184.18
		C6	NAG E	242	3.835	56.114	-21.900	1.00	184.18
	7551	06	NAG E	242	2.768	56.046	-20.979	1.00	184.18
	7552	C1	NAG E	243	2.525	57.919	-24.745	1.00	162.87
	7553	CS	NAG E	243	0.990	57.891	-24.616		
70	7554	N2	NAG E	243	0.580	57.065		1.00	162.87
					J.J00	57.000	-23.493	1.00	162.87

	3666	~~							
	7555 7556	C7 O7	NAG E NAG E	243	-0.334	57.510	-22.639	1.00	162.87
	7557	C8	NAG E	243 243	-0.848	58.623	-22.738	1.00	162.87
	7558	යි ·	NAG E	243	-0.729 0.393	56.592	-21.497	1.00	162.87
5	7559	O3	NAG E	243	-1.018	57.321 57.363	-25.904	1.00	162.87
_	7560	C4	NAG E	243	0.891	58.108	-25.842 -27.133	1.00	162.87
	7561	04	NAG E	243	0.428	57.479	-28.366	1.00 1.00	162.87
	7562	C5	NAG E	243	2.430	58.133	-27.118	1.00	162.87
	7563	O5	NAG E	243	2.904	58.707	-25.885	1.00	162.87 162.87
10	7564	C6	NAG E	243	3.044	58.927	-28.250	1.00	162.87
	7565	O 6	NAG E	243	2.770	60.311	-28.097	1.00	162.87
	7566	C1	MAN E	244	-0.169	58.185	-29.362	1.00	177.48
	7567 7568	C2	MAN E	244	-1.467	58.963	-29.047	1.00	177.48
15	7569	O2 C3	MAN E	244	-1.159	60.326	-28.837	1.00	177.48
13	7570	03	MAN E MAN E	244 244	-2.273	58.794	-30.382	1.00	177.48
	7571	C4	MAN E	244	-3.531 -1.469	59.444 59.230	-30.342	1.00	177.48
	7572	04	MAN E	244	-1.469	59.230 59.074	-31.646	1.00	177.48
	7573	C5	MAN E	244	-0.223	58.317	-32.823 -31.725	1.00 1.00	177.48
20	7574	O5	MAN E	244	0.620	58.472	-30.547	1.00	177.48
	7575	C6	MAN E	244	0.611	58.487	-33.000	1.00	177.48 177.48
	7576	O 6	MAN E	244	1.488	59.592	-32.913	1.00	177.48
	7577	C1		250	13.381	78.909	-13.725	1.00	249.71
25	7578	C2	NAG E	250	12.909	80.209	-13.049	1.00	249.71
23	7579	N2	NAG E	250	13.077	80.124	-11.608	1.00	249.71
	7580 7581	C7 O7	NAG E	250	13.987	80.876	-10.993	1.00	249.71
	7582	C8	NAG E NAG E	250	14.727	81.658	-11.592	1.00	249.71
	7583	C3	NAG E	250 250	14.097 11.429	80.733	-9.481	1.00	249.71
30	7584	O3	NAG E	250	11.000	80.446 81.693	-13.387 -12.858	1.00	249.71
	7585	C4	NAG E	250	11.216	80.427	-14.906	1.00 1.00	249.71
	7586	04	NAG E	250	9.826	80.512	-15.194	1.00	249.71 249.71
	7587	C5	NAG E	250	11.793	79.133	-15.504	1.00	249.71
25	7588	O 5	NAG E	250	13.187	78.993	-15.143	1.00	249.71
35	7589	C6	NAG E	250	11.720	79.107	-17.018	1.00	249.71
	7590	O6	NAG E	250	12.531	78.071	-17.553	1.00	249.71
	7591 7592	C1 C2	NAG E	274	17.952	58.017	0.947	1.00	232.95
	7593	N2	NAG E NAG E	274 274	17.034	57.505	2.065	1.00	232.95
40	7594	C7	NAG E	274	16.704 15.587	58.587 58.533	2.972	1.00	232.95
	7595	07	NAG E	274	14.789	57.594	3.690 3.617	1.00 1.00	232.95
	7596	C8	NAG E	274	15.307	59.699	4.627	1.00	232.95 232.95
	7597	C3	NAG E	274	17.729	56.379	2.842	1.00	232.95
45	7598	O3	NAG E	274	16.822	55.816	3.780	1.00	232.95
45	7599	C4	NAG E	274	18.227	55.288	1.888	1.00	232.95
	7600	04	NAG E	274	18.999	54.339	2.613	1.00	232.95
	7601 7602	C5	NAG E	274	19.081	55.909	0.772	1.00	232.95
	7602	O5 C6	NAG E NAG E	274	18.329	56.933	0.083	1.00	232.95
50	7604	06	NAG E	274 274	19.520 20.106	54.898 55.536	-0.274	1.00	232.95
	7605	Č1	NAG E	335	-12.841	75.891	-1.399 -12.527	1.00	232.95
	7606	C2	NAG E	335	-11.869	76.721	-12.52 <i>1</i> -11.656	1.00 1.00	244.27
	7607	N2	NAG E	335	-12.291	76.605	-10.271	1.00	244.27 244.27
	7608	C7	NAG E	335	-11.503	76.035	-9.365	1.00	244.27
55	7609	07	NAG E	335	-10.386	75.589	-9.628	1.00	244.27
	7610	C8	NAG E	335	-12,039	75.956	-7.947	1.00	244.27
	7611	C3	NAG E	335	-11.803	78.214	-12.025	1.00	244.27
	7612	O3	NAG E	335	-10.618	78.779	-11.480	1.00	244.27
60	7613 7614	C4 O4	NAG E NAG E	335 335	-11.806	78.418	-13.537	1.00	244.27
00	7615	C5	NAG E	335	-11.818	79.805	-13.844	1.00	244.27
	7616	O5	NAG E	335	-13.044 -12. 94 0	77.739 76.310	-14.108 -13.013	1.00	244.27
	7617	C6	NAG E	335	-13.184	76.310 77.982	-13.913 -15.605	1.00	244.27
	7618	06	NAG E	335	-14.397	78.652	-15.605	1.00 1.00	244.27
65	7619	C1	NAG E	340	-14.368	66.477	8.751	1.00	244.27 249.77
	7620	C2	NAG E	340	-13.779	65.349	9.574	1.00	249.77
	7621	N2	NAG E	340	-13.415	64.233	8.721	1.00	249.77
	7622	C7	NAG E	340	-12.195	63.711	8.818	1.00	249.77
70	7623 7624	O7	NAG E	340	-11.344	64.132	9.612	1.00	249.77
, 0	/ 024	C8	NAG E	340	-11.863	62.550	7.900	1.00	249.77

	7625 7626 7627 7628	C3 O3 C4	NAG E NAG E NAG E	340 -14.783 340 -14.195 340 -15.166	64.920 63.909 66.132	10.636 11.453	1.00 1.00	249.77 249.77
5	7628 7629	O4 · C5	NAG E	340 -16.238	65.759	11.500 12.355	1.00	249.77
•	7630	O5	NAG E	340 -15.575	67.356	10.636	1.00	249.77
	7631	C6	NAG E	340 -14.610	67.605	9.591	1.00	249.77
	7632	06	NAG E NAG E	340 -15.666	68.648	11.433	1.00	249.77
	7633	C1	NAG E NAG E	340 -15.300	69.781	10.659	1.00 1.00	249.77
10	7634	C2	NAG E	366 -12.398	52.150	-11.858	1.00	249.77
	7635	N2	NAG E	366 -11.828	51.489	-13.095	1.00	131.22
	7636	C7	NAG E	366 -11.760 366 -10.652	52.463	-14.162	1.00	131.22
	7637	07	NAG E		53.170	-14.339	1.00	131.22 131.22
15	7638	C8	NAG E	366 -9.658 366 -10,642	53.028	-13.631	1.00	131.22
15	7639	C3	NAG E	366 -12.712	54.189	-15.474	1.00	131.22
	7640	О3	NAG E	366 -12.088	50.337	-13.517	1.00	131.22
	7641	C4	NAG E	366 -12,958	49.646 49.373	-14.588	1.00	131,22
	7642 7643	04	NAG E	366 -13.982	48.430	-12.351	1.00	131,22
20	7644	C5	NAG E	, 366 -13.414	50.137	-12.735	1.00	131,22
~0	7645	O5	NAG E	366 -12.496	51.204	-11.096	1.00	131.22
	7646	C6 Q6	NAG E	366 -13.478	49.261	-10.795 -9.862	1.00	131.22
	7647	C1	NAG E	366 -13.939	49.998	-9.862 -8.740	1.00	131.22
	7648	C2	NAG E	367 -13.682	47.077	-12.614	1.00	131.22
25	7649	N2	NAG E	367 -14.975	46.261	-12.520	1.00	245.35
	7650	C7	NAG E NAG E	367 -15.776	46.701	-11.394	1.00 1.00	245.35
	7651	07	NAG E NAG E	367 -16.904	47.372	-11.610	1.00	245.35
	7652	C8	NAG E	367 -17.315	47.646	-12,739	1.00	245.35
20	7653	C3	NAG E	367 -17.698	47.808	-10.389	1.00	245.35
30	7654	О3	NAG E	367 -14.620 367 -15.804	44.778	-12.391	1.00	245.35
	7655	C4	NAG E		43.995	-12.351	1.00	245.35 245.35
	7656	O4	NAG E	367 -13.757 367 -13.340	44.354	-13.584	1.00	245.35 245.35
	7657	C5	NAG E	367 -12,529	43.005	-13.423	1.00	245.35
35	7658	O5	NAG E	367 -12.935	45.270	-13.701	1.00	245,35
J)	7659	C6	NAG E	367 -11.710	46.662	-13.772	1.00	245.35
	7660	O6	NAG E	367 -11,792	44.973 46.031	-14.941	1.00	245.35
				1 02	46.031	-15.884	1.00	245.35

Table 6. Atomic coordinates of PhFcεRIα₁₋₁₇₂, Form T2

				minate	s of PhFc	εRΙα ₁₋₁₇₂ , Fo	rm Tr			
	AT NU	OM IMBER	TIOM	ESIDUE						
	_ 1					<u> </u>	Υ			
	5 2		B LY	rs c	4 1	5.063 45 £			OCC B	
			בי בי	S C	4 17	7.178	227	50.293	1.00	•
	4	C	E LY		4 18	3.081 43.7		49.692	444 270,00	
	5 6	N	Z LY	SC	4 19	.152 ∡os		50.766 50.151	1.00 240.56	
	10 7	C O		S C		.054 42.2 .440 44.6	O į	51.173	240.56	
	8	N			4 14			48.479	240.56	
	9	C.	LY:	S C	4 14,	039 46.6	06 (14	18.972	4 A- E-10.4D	
	10 11	N	PR	0 C	4 15. 5 13	077 45 79		19.935	1.00 248.46	
	15 12	CE CA	' PRO	O C	5 13.	962 44.90)2		248.46	
	13	CB	1 176	Ç Č	5 13.	330	.9 4	C COF	240.49	
	14	CG) (5 12.4	101 44 63	6 7	6.448	1.00 226.60 1.00 240.49	
	15 16	C	PRO) C	5 13.1 5 14.3	89 45.88	1 7	5.543 1	.00 226.60	
	20 17	O N	PRO) C	5 14.3 5 15.4	~ ~	3 49		.00 226.60	
	18	CA	LYS	C	6 14.0	67 43,532 22 41.831	1 45	. 400	.00 240.49 .00 240.40	
	19	CB	LYS LYS	C	6 14.9	32 40 986	70	.280 _{1.}	m 240.49	
	20 21	CG	LYS	-	6 15.67 6 16.70	70 40 017	. 44	.518 1.	00 200.38	
:	25 22	CD CE	LYS	С	6 16.70 6 17.53	00.100	44	700	249.33	
	23	NZ	LYS	C ,	6 18.56		45.	692	00 249.33	
	24 25	С	LYS LYS	_	19.47	1 36 732	44.	943		
	25 26	0	LYS	C A		8 40 207	45. 43.	855 1.0	0 249.33	
3	30 27	N CA	VAL	c 3			43.	766	0 200.38	
	28	CB	VAL		13.799		42.1	190 10	200.36	
	29 30	CG1	VAL (C 7 C 7	14.155	40.623	41.0	⁷⁵² 1.0		
_	24	CG2	VAL (3 7	13.207 14.108	40.181	39.7 38.6	4.0	D 175 84	
3.	5 32	CO	VAL	7	14.153		39.9	45 1.00 44 1.00	175.84	
	33	Ň	VAL (SER (15.316	38.431 38.073	40.8	84 1.00	173.04	
	34 35	CA	SER C		13.132	37.584	40.74	⁴⁶ 1.00		
	36	CB	SER C		13.318 12.487	36.148	40.88 40.72		212.94	
40) 37	OG C	SER C	8	11.148	35.385	41.75		212.94	
	38	0	SER C SER C	-	12.886	35.858 35. 75 5	41.80	1.00	203.15	
	39 40	N	LEU C	8 9	12.169	36.508	39,30	7 1.00	203.15 212.94	
	41	. CA CB	LEU C	9	13.330 12.955	34.593	38.64 38.83	1.00	212.94	
45		CG	LEU C	9	14.150	34.137	37.49		249.13	
	43	CD1	TEN C	9	14.916	34.163 35.465	36.540	1.00	249.13	
	44 45	CD2	LEU C	9 9	. 15.771	35.258	36.269		143.92 143.92	
	46	CO	LEU C	9	13.966 12.395	36.637	35.022 36.063	1.00	143,92	
50	47	Ň	LEU C	9	12.617	32.728 31.964	37.507	1.00 1.00	143.92	
	48 49	CA	ASN C	10	11.667	32.389	38.445	1.00	249.13 249.13	
	50	CB	ASN C	10 10	11.095	31.064	36.451 36.336	1.00	171.60	
55	51	CG OD1	ASN C	10	9.847 9.428	30.927	36.3 <u>26</u> 37.201	1.00 1.00	171.60	
55	52	ND2	ASN C ASN C	10	10.163	29.487 28.684	37.375	1.00	226.23	
	53 54	C	ASN C	10 10	8.251	29.146	37.948	1.00	226.23 226.23	
	55	0	ASN C	10	10.724	30.744	36.870 34.882	1.00	226.23	
60	56	N CD	PRO C	11	9.817 11.452	31.353	34.315	1.00 1.00	171.60	
60	57	CA	PRO C	11	11.153	29.806 29.449	34.238	1.00	171.60	
	58 59	CB	PRO C	11	12.551	28.981	32.850	1.00	202.18 161.79	
	60	CG	PRO C	11 11	13.028	28.248	34.761 33.517	1.00	202.18	
45	61	CO	PRO C	11	11.770 13.687	28.086	32.742	1.00 1.00	161.79	
65	62	N	PRO C PRO C	11	13.753	29.788 31.010	35.394	1.00	161.79	
	63 64	CD	PRO C	12	14.598	29.101	35.265	1.00	202.18 202.18	
	65	CA CB	PRO C	12 12	14.562 15.721	27.680	36.104 36.472	1.00	182.42	
		OB	PRO C	12	16.307	29.778	36.762	1.00 1.00	171.80	
				•		28.681	37.663	1.00	182.42	
									171.80	

	136	СВ	GLU C	20 ·	12.136	30.161	25.259	1.00	170 =
	137	CG	GLU C	20	12.994	29.290	24.335	1.00	176.57 176.57
	138	CD	GLU C	20	14.115	28.594	25.077	1.00	176.57
5	139 140	OE1 OE2	GLU C	20	14.898	29.282	25.777	1.00	176.57
,	141	C	GLU C	20	14.217	27.356	24.959	1.00	176.57
	142	ŏ	GLU C	20 20	10.297 10.532	31.833	25.582	1.00	154.05
	143	Ň	ASN C	21	9.550	33.032 31.365	25.419 26.587	1.00	154.05
	144	CA	ASN C	21	8.957	32.290	27.559	1.00 1.00	173.20
10	145	СВ	ASN C	21	7.446	32.074	27.682	1.00	173.20 249.69
	146	CG	ASN C	21	6.794	31.675	26.378	1.00	249,69
	147 148	OD1 ND2	ASN C	21	7.014	32.277	25.326	1.00	249.69
	149	C	ASN C ASN C	21 21	5.961 9.559	30.647	26.472	1.00	249.69
15	150	ŏ	ASN C	21	9.892	32.227 31.148	28.975	1.00	173.20
	151	Ň	VAL C	22	9.661	33.393	29.474 29.617	1.00 1.00	173.20
	152	CA	VAL C	22	10.209	33.508	30.964	1.00	186.44 186.44
	153	CB	VAL C	22	11.664	34.016	30.926	1.00	163.28
20	154 155	CG1	VAL C	22	11.701	35.486	30.538	1.00	163.28
20	156	CG2 C	VAL C VAL C	22	12.315	33.802	32.273	1.00	163.28
	157	ŏ	VAL C VAL C	22 22	9.379 8.852	34.489	31.797	1.00	186.44
	158	Ň	THE	23	9.289	35.463 34.241	31.271 33.102	1.00	186.44
~-	159	CA	THR C	23	8.512	35.092	34.014	1.00 1.00	165.76 165.76
25	160	CB	THR C	23	7.425	34.263	34.728	1.00	249.09
	161	OG1	THR C	23	6.671	33.521	33.760	1.00	249.09
	162 163	CG2	THR C	23	6.492	35.177	35.511	1.00	249.09
	164	CO	THR C THR C	23 23	9.348	35.780	35.098	1.00	165.76
30	165	Ň	LEU C	23 24	10.061 9.239	35.119 37.099	35.850	1.00	165.76
	166	CA	LEU C	24	9.990	37.842	35.195 36.206	1.00 1.00	173.95
	167	CB	LEU C	24	10.661	39.079	35.589	1.00	173.95 128.36
	168	CG	LEU C	24	11.163	39.097	34.140	1.00	128.36
35	169 170	CD1	LEU C	24	12.080	40.307	33.939	1.00	128.36
33	171	CD2 C	LEU C	24	11.903	37.824	33.821	1.00	128.36
	172	ŏ	LEU C	24 24	9.089 8.276	38.297 39.207	37.365	1.00	173.95
	173	Ň	THR C	25	9.249	37.669	37.208 38.526	1.00 1.00	173.95
40	174	CA	THR C	25	8.463	37.995	39.717	1.00	172.54 172.54
40	175	СВ	THR C	25	8.096	36.712	40.504	1.00	195.25
	176	OG1	THR C	25	7.369	35.824	39.645	1.00	195.25
	177 178	CG2 C	THR C THR C	25	7.244	37.045	41.724	1.00	195.25
	179	ŏ	THR C	25 25	9.253 10.427	38.923 38.681	40.636	1.00	172.54
45	180	Ň	CYS C	26	8.610	39.978	40.895 41.130	1.00 1.00	172.54
	181	CA	CYS C	26	9.269	40.937	42.025	1.00	199.84 199.84
	182	Ç	CYS C	26	9.272	40.407	43.458	1.00	199.84
	183	0	CYS C	26	8.303	39.775	43.889	1.00	199.84
50	184 185	CB SG	CYS C CYS C	26 06	8.556	42.292	41.955	1.00	211.93
-	186	N	ASN C	26 27	9.426 10.358	43.668	42.769	1.00	211.93
	187	CA	ASN C	27	10.531	40.673 40.203	44.186 45.564	1.00	249.36
	188	CB	ASN C	27	11.176	41.291	46.437	1.00	249.36
55	189	CG	ASN C	27	11.614	40.764	47.804	1.00	249.69 249.69
55	190	OD1	ASN C	27	12.279	39.728	47.907	1.00	249.69
	191 192	ND2 C	ASN C ASN C	27	11.246	41.481	48.858	1.00	249.69
	193	ŏ	ASN C	27 27	9.245 8.484	39.705	46.225	1.00	249.36
	194	Ň	GLY C	28	9.029	40.481 38.395	46.815 46.116	1.00	249.36
60	195	CA	GLY C	28	7.858	37.746	46.116 46.685	1.00 1.00	249.69 249.69
	196	C	GLY C	28	7.872	36.313	46.199	1.00	249.69
	197	0	GLY C	28	7.839	36.074	44.991	1.00	249.69
	198 199	N CA	ASN C	29	7.927	35.361	47.129	1.00	249.69
65	200	CA CB	ASN C ASN C	29 20	7.980	33.942	46.771	1.00	249.69
	201	CG	ASN C	29 29	8.454 8.804	33.111	47.988	1.00	249.69
	202	OD1	ASN C	29	8.854	31.655 31.278	47.627 46.450	1.00	249.69
	203	ND2	ASN C	29	9.055	30.840	48.650	1.00 1.00	249.69 249.69
70	204	C	ASN C	29	6.655	33.386	46.224	1.00	249.69 249.69
/U	205	0	ASN C	29	6.633	32.784	45.140	1.00	249.69

							4.00	040.60
000	N	ASN C	30°	5.554	33.594	46.946	1.00 1.00	249.69 249.69
206	CA	,,,,,,	30	4.270	33.055	46.497	1.00	249.69
207 208	CB		30	3.852	31.902	47.424 47.372	1.00	249.69
209	ČĞ	ASN C	30	4.822	30.717	48.410	1.00	249.69
5 210	OD1	ASN C	30	5.230	30.182 30.299	46.163	1.00	249.69
211	ND2	ASN C	30	5.186	34.055	46.361	1.00	249.69
212	C	ASN C	30	3.119 2.662	34.325	45.248	1.00	249.69
213	0	ASN C PHE C	30 31	2.650	34.602	47.482	1.00	249.69
214	N	PHE C PHE C	31	1.531	35.546	47.446	1.00	249.69
10 215	CA	PHE C	31	0.361	35.003	48.290	1.00	249.52 249.52
216	CB CG	PHE C	31	-0.075	33.609	47.903	1.00	249.52 249.52
217	CD1	PHE C	31	0.636	32.498	48.348 47.071	1.00 1.00	249.52
218 219	CD2	PHE C	31	-1.176	33.411	47.966	1.00	249.52
15 220	CE1	PHE C	31	0.261	31.211 32.128	46.684	1.00	249.52
221	CE2	PHE C	31	-1.557	31.026	47.132	1.00	249.52
222	CZ	PHE C	31	-0.838 1.872	36.984	47.884	1.00	249.69
223	č	PHE C PHE C	31 31	2.350	37.22	49.003	1.00	249.69
224	0	PHE C PHE C	32	1.605	37.936	46.986	1.00	249.62
20 225	N CA	PHE C	32	1.872	39.354	47.227	1.00	249.62 249.69
226	CB	PHE C	32	2.862	39.873	46.176	1.00 1.00	249.69
227 228	CG	PHE C	32	3.487	41.203	46.520 47.611	1.00	249.69
229	CD1	PHE C	32	4.351	41.325 42.334	45.741	1.00	249.69
25 230	CD2	PHE C	32	3.224	42.554 42.554	47.918	1.00	249.69
231	CE1	PHE C	32	4.948	43.566	46.039	1.00	249.69
232	CE2	PHE C	32	3.814 4.678	43.673	47.130	1,00	249.69
233	CZ	PHE C	32 32	0.569	40.161	47.176	1.00	249.62
234	C	PHE C PHE C	32	-0.470	39.650	46.738	1.00	249.62
30 235	0 N	GLU C	33	0.636	41.424	47.595	1.00	238.93 238.93
236	CA	GLU C	33	-0.554	42.273	47.631	1.00 1.00	249.69
237 238	CB	GLU C	33	-0.811	42,705	49.079 49.339	1.00	249.69
239	CG	GLU C	33	-2.234	43.193 42.246	48.762	1.00	249.69
35 240	CD	GLU C	33	-3.285	41.010	48.947	1.00	249.69
241	OE1	GLU C	33	-3.144 -4.250	42.733	48.124	1.00	249.69
242	QE2	GLU C	33 33	-0.613	43.512	46.721	1.00	238.93
243	C	GLU C	33	-1.589	43.716	45.998	1.00	238.93
244	0	VAL C	34	0.420	44.344	46.762	1.00	237.42 237.42
40 245	N GA	VAL C	34	0.452	45.563	45.959	1.00 1.00	249.69
246 247	CB	VAL C	34	1.760	46.350	46.235 45.447	1.00	249.69
248	CG1	VAL C	34	1.775	47.644	47.726	1.00	249.69
249	CG2	VAL C	34	1.875	46.644 45.376	44,447	1.00	237.42
45 250	С	VAL C	34	0.284 0.665	44.351	43.880	1.00	237.42
251	0	VAL C	34 35	-0.305	46.386	43.812	1.00	249.64
252	N	SER C SER C	35 35	-0.535	46.390	42.370	1.00	249.64
253	CA CB	SER C SER C	35	-1.976	46.787	42.058	1.00	249.69 249.69
254 50 255		SER C	35	-2.186	48.165	42.327	1.00 1.00	249.64
256 256	_	SER C	35	0.403	47.409	41.729 40.504	1.00	249.64
257 257	_	SER C	35	0.418	47.573 48.101	42.573	1.00	249.69
258	N N	SER C	36	1.171	49,109	42.112	1.00	249.69
259	CA	SER C	36	2.129 2.054	50.374	42.987	1.00	249.69
55 260		SER C	36 36	2.599	50.160	44.280	1.00	249.69
261		SER C	36	3.555	48,551	42.130		249.69 249.69
262		SER C	36	4.261	48.626	43.142		198.99
263 264		THR C	37	3.961	47.977	40.999		198.99
60 26	·	THR C	37	5.286	47.408	40.863 40.697		176.65
26		THR C	37	5.205	45.867	41.840		176.65
26	7 OG1	THR C	37	4.557	45.280 45.275	40.573		176.65
26	8 CG2	THR C	37	6.597 5.905	48.053	39.632	1.00	198.99
26	9 C	THR C		5.232	48.246	38.619	1.00	198.99
65 27		THR C		7.182	48.400	39.72		249.69 249.69
27		LYS C		7.865	49.041	38.60		249.69 249.38
27		LYS	38	8.609	50.287	39.10		249.38
27 27		LYS C	38		51.314	39.79 40.30		249.38
	75 CD	LYS C	38	8.467	52,537	40.00		
				•				

	276	CE	LYS C	38	7.527	53.572	40.020	4.00	
	277	NZ.	LYS C	38	8.240	53.572 54.792	40.930 41.414	1.00	249.38
	278	C	LYS C	38	8.837	48.092	37.894	1.00 1.00	249.38 249.69
~	279	0 .	LYS C	38	9.473	47.247	38.519	1.00	249.69
5	280	N	TRP C	39	8.933	48.221	36.576	1.00	205.23
	281 282	CA	TRP C	39	9.837	47.391	35.790	1.00	205.23
	283	CB CG	TRP C TRP C	39	9.052	46.417	34.916	1.00	163.48
	284	CD2	TRP C	39 39	8.273 8.795	45.376	35.653	1.00	163.48
10	285	CE2	TRP C	39	7.715	44.365 43.525	36.525	1.00	163.48
	286	CE3	TRP C	39	10.069	44.083	36.893 37.032	1.00 1.00	163.48
	287	CD1	TRP C	39	6.939	45.125	35.542	1.00	163,48 163,48
	288	NE1	TRP C	39	6.591	44.013	36.278	1.00	163.48
15	289	CZ2	TRP C	39	7.866	42.419	37.737	1.00	163.48
15	290	CZ3	TRP C	39	10.225	42.976	37.881	1.00	163.48
	291 292	CH2 C	TRP C	39	9.125	42.162	38.220	1.00	163.48
	293	ŏ	TRP C TRP C	39 39	10.637	48.332	34.908	1.00	205.23
	294	ŭ	PHE C	40	10.076 11.947	49.233 48.138	34.280	1.00	205.23
20	295	CA	PHE C	40	12.800	49.016	34.857 34.034	1.00	127.08
	296	СВ	PHE C	40	13.686	49.895	34.930	1.00 1.00	127.08
	297	CG	PHE C	40	12.922	50.766	35.900	1.00	249.69 249.69
	298	CD1	PHE C	40	12.431	50.242	37.097	1.00	249.69
25	299	CD2	PHE C	40	12.724	52,121	35.630	1.00	249.69
25	300 301	CE1	PHE C	40	11.762	51.055	38.010	1.00	249.69
	302	CE2 CZ	PHE C PHE C	40	12.054	52.941	36.539	1.00	249.69
	303	C	PHE C	40 40	11.574	52.408	37.731	1.00	249.69
	304	ŏ	PHE C	40	13.714 14.938	48.294 48.204	33.012	1.00	127.08
30	305	N	HIS C	41	13.118	47.801	33.191 31.936	1.00 1.00	127.08
	306	CA	HIS C	41	13.846	47.101	30.884	1.00	117.94
	307	СВ	HIS C	41	12.846	46.566	29.848	1.00	117.94 198.34
	308	CG	HIS C	41	13.482	45.817	28.723	1.00	198.34
35	309	CD2	HIS C	41	13.214	45.791	27.395	1.00	198.34
22	310	ND1	HIS C	41	14.515	44.930	28.924	1.00	198.34
	311 312	CE1 NE2	HIS C	41	14.856	44.390	27.769	1.00	198.34
	313	C	HIS C HIS C	41 41	14.082	44.895	26.826	1.00	198.34
	314	ŏ	HIS C	41	14.863 14.509	48.015 48.859	30.192	1.00	117.94
40	315	Ň	ASN C	42	16.135	47.813	29.389 30.481	1.00 1.00	117.94
	316	CA	ASN C	42	17.216	48.618	29.912	1.00	147.15 147.15
	317	CB	ASN C	42	17.135	48.679	28.370	1.00	208.25
	318	CG	ASN C	42	17.652	47.411	27.699	1.00	208.25
45	319 320	OD1	ASN C	42	17.253	46.309	28.074	1.00	208.25
43	321	ND2 C	ASN C ASN C	42	18.527	47.562	26.702	1.00	208.25
	322	ŏ	ASN C	42 42	17.140	50.019	30.506	1.00	147.15
	323	Ň	GLY C	43	17.627 16.527	50.986 50.115	29.917 31.683	1.00	147.15
	324	CA	GLY C	43	16.372	51.400	32.344	1.00	230.72
50	325	С	GLY C	43	15.019	52.031	32.048	1.00 1.00	230.72 230.72
	326	0	GLY C	43	14.369	52.590	32.933	1.00	230.72
	327	N	SER C	44	14.596	51.937	30.790	1.00	208.53
	328	CA	SER C	44	13.320	52.490	30.334	1.00	208.53
55	329 330	CB OG	SER C	44	13.133	52,231	28.83	1.00	178.10
-	331	c	SER C SER C	44 44	14.168	52.830	28.070	1.00	178.10
	332	ŏ	SER C	44	12.146 11.961	51.881 50.670	31.079	1.00	208.53
	333	N	LEU C	45	11.338	52.719	31.066 31.713	1.00	208.53
~	334	CA	LEU C	45	10.186	52.214	32,442	1.00 1.00	211.15 211.15
60	335	СВ	LEU C	45	9.346	53.372	32.985	1.00	239.89
	336	CG	LEU C	45	8.132	52.948	33.821	1.00	239.89
	337	CD1	LEU C	45	8.571	52.034	34.952	1.00	239.89
	338 339	CD2	LEU C	45	7.433	54.178	34.368	1.00	239.89
65	340	C	LEU C	45 45	9.330	51.325	31.540	1.00	211.15
	341	Ň	SER C	45 46	9.278 8.660	51.528	30.323	1.00	211.15
	342	ČA	SER C	46 46	8.669 7.826	50.339	32.143	1.00	166.46
	343	CB	SER C	46	8.138	49.404 47.964	31.400 31.815	1.00	166.46
70	344	OG	SER C	46	7.394	47.032	31.043	1.00 1.00	249.69
70	345	С	SER C	46	6.345	49.671	31.608	1.00	249.69 166.46
						•			.50.70

			arn 6	46 ·	5.973	50.451	32.488	1.00	166.46 202.45
3	146	_			5.512	48.996	30.813	1.00	202.45
3	347	• •	GLU C	47	4.064	49.168	30.864	1.00 1.00	249.69
	348	CA	GLU C	47	3.485	49.010	29.458	1.00	249.69
_ ;	349	CB .	GLU C	47	4.000	50.047	28.469 27.078	1.00	249.69
	350	CD CD	GLU C	47	3.429	49.860	26.462	1.00	249.69
	351	OE1	GLU C	47	3.693	48.805	26.600	1.00	249.69
	352	OE2	GLU C	47	2.715	50.769 48.271	31.832	1.00	202.45
	353 354	C	GLU C	47	3.296	48.506	32.090	1.00	202.45
	35 4 355	ŏ	GLU C	47	2.108 3.948	47.243	32.361	1.00	214.28
10	356	N	GLU C	48	3.264	46.372	33.301	1.00	214.28
	357	CA	GLU C	48	3.882	44.973	33.294	1.00	197.36
	358	CB	GLU C	48 48	3.286	44.027	34.340	1.00	197.36 197.36
	359	CG	GLU C	48	1.825	43.715	34.097	1.00 1.00	197.36
15	360	CD	GLU C	48	1.535	42.984	33.130	1.00	197.36
	361	OE1	GLU C	48	0.964	44.203	34.866 34.702	1.00	214.28
	362	OE2 C	GLU C	48	3.343	46.977	34.995	1.00	214.28
	363	ő	GLU C	48	4.236	47.788	35.557	1.00	211.95
20	364	N	THR C	49	2.398	46.584 47.069	36.932	1.00	211.95
20	365 366	CA	THR C	49	2.335	48.003	37.123	1.00	249.69
	367	СВ	THR C	49	1.126	47.327	36.706	1.00	249.69
	368	OG1	THR C	49	-0.069 1.305	49.278	36.301	1.00	249.69
	369	CG2	THR C	49	2.220	45.895	37.901	1.00	211.95 211.95
25	370	С	THR C	49 49	2.631	45.988	39.055	1.00	207.90
	371	0	THR C	50	1.650	44.797	37.421	1.00	207.90
	372	N.	ASN C	50	1.502	43.601	38.234	1.00 1.00	210.82
	373	CA	ASN C	50	0.856	42.486	37.403	1.00	210.82
••	374	CB CG	ASN C	50	0.443	41.295	38.245 39.365	1.00	210.82
30	375	OD1	ASN C	50	0.925	41.126	37,705	1.00	210.82
	376	ND2	ASN C	50	-0.437	40.456 43.187	38.670	1.00	207.90
	377 378	C	ASN C	50	2.914	43.479	37.978	1.00	207.90
	379	ō	ASN C	50	3.888 3.036	42.509	39.808	1.00	249.50
35	380	N	SER C	51	4.352	42.086	40.286	1.00	249.50
55	381	CA	SER C	51 51	4.260	41.569	41.728	1.00	249.69 249.69
	382	CB	SER C	51	3.632	40.295	41.780	1.00	249.50
	383	og.	SER C SER C	51	4.994	41.012	39.395	1.00 1.00	249.50
	384	Ç	SER C	51	6.196	40.775	39.483 38.544	1.00	228.11
40	385	О N	SER C	52	4.195	40.367	37.645	1.00	228.11
	386	CA	SER C	52	4.705	39.328 38.049	37.741	1.00	168.18
	387 388	CB	SER C	52	3.867	37.491	39.042	1.00	168.18
	389	OG	SER C	52	3.908	39.783	36.194	1.00	228.11
45	390	C	SER C	52	4.726 3.692	39.843	35.528	1.00	228.11
73	391	0	SER C	52 53	5.919	40.096	35.708		153.71 153.71
	392	N _.	LEU C		6.111	40.542	34.332		123.91
	393	CA	LEU C		7.219	41.594	34.278		123.91
	394	CB CB	LEU C		7.891	41.882	32.939 31.823		123.91
50		· CD1	LEU		6.841	42.018	33.084		123.91
	396	CD2	LEU		8.744	43.157 39.373	33.439		153.71
	397 398	C	LEU C	53		38.887	33.46	1 1.00	153.71
	399	ō	LEU (38.918	32.65	5 1.00	221.05
5.	5 400	N	ASN C		·	37.804	31.77		221.05 192.59
<i>J</i> .	401	CA	ASN			37.081	31.43		192.59
	402	СВ	ASN (36.312	32.60		192.59
	403	CG	ASN (-		35.511	33.21		192.59
	404	OD1		-		36.548	32.92		221.05
6	0 405	ND2	ASN	_	4 6.477	38.221	30.49 30.09		221.05
	406	CO			4 6.451	39.391	29.87		249.69
	407	N		•	5 7.116	37.234	28.6		249.69
	408	CA	ILE	C 5	5 7.850	37.402 37.380	28.8		131.97
	409	CB	iLE	C 5	9.374	37.380 36.988	27.5		131.97
•	65 410 411	ČG2	2 ILE	C	55 10.103		29.3	80 1.00	
	412	CG	1 ILE	-	55 9.822 55 11.301	38.863	29.6	65 1.00	
	413	CD	1 ILE	•			27.7		
	414	Ç	ILE	_	55 7.468 55 7.742		28.0	48 1.00	249.68
	70 415	0	ILE	C	JJ 7.1. T				

						36.531	26.595	1.00	201.86
4	16	N	VAL C	58	6.829	35.474	25.687	1.00	201.86
	17	CA	VAL C	56	6.422	35.759	25.089	1.00	231.54
	18	CB	VAL C	56	5.043	34.468	24.565	1.00	231.54
	19	CG1	VAL C	56	4.431	36.385	26.138	1.00	231.54
	20	CG2	VAL C	56	4.144 7.454	35.345	24.578	1.00	201.86
	21	С	VAL C	56	8.595	35.775	24.747	1.00	201.86
	22	0	VAL C	56	7.056	34.758	23.451	1.00	157.94
	23	N	ASN C	57	7.953	34.542	22.310	1.00	157.94
	124	CA	ASN C	57 67	7.179	34,657	20.994	1.00	249.57
	425	СВ	ASN C	57 57	6,212	33.499	20.793	1.00	249.57 249.57
	426	CG	ASN C	57	6.593	32.333	20.911	1.00	249.57 249.57
	427	OD1	ASN C	57	4.958	33.812	20.488	1.00	157.94
	428	ND2	ASN C	57	9.147	35.472	22.324	1.00 1.00	157.94
	429	Ç	ASN C	57	9.103	36.592	21.825	1.00	146.95
	430	0	ALA C	58	10.213	34.960	22.924	1.00	146.95
	431	N	ALA C	58	11.477	35.658	23.112 23.796	1.00	132.39
	432	CA	ALA C	58	12.467	34.717	21.878	1.00	146.95
	433	CB C	ALA C	58	12.122	36.270	21.014	1.00	146.95
00	434	Ö	ALA C	58	12.657	35.566	21.816	1.00	135.91
20	435	N	LYS C	59	12.087	37.596	20.710	1.00	135.91
	436	CA	LYS C	59	12.680	38.350	20.270	1.00	248.43
	437	CB	LYS C	59	11.742	39.483	19.795	1.00	248.43
	438	CG	LYS C	59	10.375	39.002 40.157	19.482	1.00	248.43
25	439	CD	LYS C	59	5, 126	39.641	19.094	1.00	248.43
23	440 441	CE	LYS C	59	8.053	40.738	18.771	1.00	248.43
	442	NZ	LYS C	59	7.100	38.928	21.228	1.00	135.91
	443	C	LYS C	59	13.986	39.415	22.354	1.00	135.91
	444	0	LYS C	59	14.052	38.866	20.406	1.00	130.99
30	445	N	PHE C	60	15.020 16.330	39.375	20.784	1.00	130.99
50	446	CA	PHE C	60	17.171	39.581	19.523	1.00	226.68 226.68
	447	CB	PHE C	60 60	17.469	38.309	18.781	1.00	226.68
	448	CG	PHE C PHE C	60	17.704	38.327	17.410	1.00 1.00	226.68
	449	CD1	PHE C PHE C	60	17.535	37.093	19.458	1.00	226.68
35	450	CD2	PHE C	60	17.998	37.156	16.724	1.00	226.68
	451	CE1	PHE C	60	17.829	35.919	18.782 17.411	1.00	226.68
	452	CE2	PHE C	60	18.061	35.951	21.597	1.00	130.99
	453	CZ	PHE C	60	16.296	40.672	22.439	1.00	130.99
40	454	CO	PHE C	60	17.171	40.914	21.338	1.00	229.15
40	455	Ň	GLU C	61	15.289	41.507	22.028	1.00	229.15
	456	CA	GLU C	61	15.136	42.789 43.603	21.363	1.00	236.43
	457 458	CB	GLU C	61	14.021	43.926	19.878	1.00	236.43
	450 459	ČĞ	GLU C	61,		42.686	19.003	1.00	236.43
45	460	CD	GLU C	61	14.424	41.786	19.062		236.43
73	461	OE1	GLU C	61	13.554	42.616	18.250		236.43
	462	OE2	GLU C		15.423 14.832	42.608	23.508		229.15
	463	С	GLU C			43,491	24.316		229.15 169.19
	464	0	GLU C			41.456	23.849		169.19
50	465	N	ASP C			41.142	25.23		219.70
•	466	CA	ASP C			39.884	25.310		219.70
	467	CB				39.951	24.41		219.70
	468	CG	ASP C			41.064	24.22 23.91		219.70
	_ 469	OD1	ASP (6		38.891	26.06		169.19
55		OD2	ASP			40.932	27.28		169.19
	471	CO	ASP	-	2 15.152	41.049	25.40		159.66
	472	N	SER		3 16.289	40.608	28.08		159.66
	473	CA	SER		3 17.564	40.400	25.08		141.40
-	474	CB	SER	C 6	3 18.659	39.965 38.774	24.39		141.40
6	0 475 476	OG	SER	C 6	33 18.325	41.730	26.7		159.66
		Č	SER	C 6	3 17.962	40 740	26.0		159.66
	477 478	ŏ	SER	-	63 18.006	44 700	28.0	09 1.00	163.83
	479	Ň	GLY	_	64 18.242	10.074	28.6	41 1.00	163.83
4	5 480	CA	GLY	C	64 18.620	40.070	30.1	54 1.00	
U	481	C	GLY	•	64 18.666		30.7		
	482	0	GLY	_	64 18.652 65 18.719		30.7		
	483	N	GLU	C		44 400	32.1		
	484	CA	GLU	C	65 18.792 65 19.859		32.3	390 1.00	240.20
-	70 485	CB	GLU	J					

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	486	CG	GLU C	65 ·	19.972	45.990	. 33.800	1.00	246.00
	487	CD	GLU C	65	20.739	47.294	33.859	1.00	246.28 246.28
	488	OE1,	GLU C	65	20.270	48.276	33.250	1.00	246.28
5	489	OE2 ·	GLU C	65	21.806	47.341	34.506	1.00	246.28
J	490 491	C	GLU C	65	17.444	44.883	32.727	1.00	155.20
	491	0 N	GLU C TYR C	65	16.907	45.897	32.306	1.00	155.20
	493	CA	TYR C	66 66	16.899 15.614	44.149	33.692	1.00	218.21
	494	CB	TYR C	66	14.600	44.507 43.380	34.299	1.00	218.21
10	495	ČĞ	TYR C	66	14.195	43.050	34.131 32.722	1.00	195.34
	496	CD1	TYR C	66	15.027	42.319	31.889	1.00 1.00	195.34
	497	CE1	TYR C	66	14.607	41.929	30.619	1.00	195.34
	498	CD2	TYR C	66	12.934	43.398	32.250	1.00	195.34 195.34
1.5	499	CE2	TYR C	66	12.505	43.016	30.985	1.00	195.34
15	500	CZ	TYR C	66	13.342	42.277	30.175	1.00	195.34
	501	ОН	TYR C	66	12.896	41.868	28.938	1.00	195.34
	502 503	C	TYR C	66	15.691	44.815	35.795	1.00	218.21
	504	Ň	TYR C LYS C	66	16.721	44.584	36.431	1.00	218.21
20	505	CA	LYS C	67 67	14.577	45.311	36.350	1.00	178.65
	506	CB	LYS C	67	14.467 15.471	45.652 46.748	37.782	1.00	178.65
	507	CG	LYS C	67	15.399	47.981	38.152 37.275	1.00	172.69
	508	CD	LYS C	67	16.474	48.976	37.275 37.663	1.00 1.00	172.69
	509	CE	LYS C	67	16.722	50.003	36.565	1.00	172.69
25	510	NZ	LYS C	67	17.749	51.022	36.952	1.00	172.69 172.69
	511	С	LYS C	67	13.078	46.103	38.229	1.00	172.65
	512	0	LYS C	67	12.289	46.623	37.437	1.00	178.65
	513	N	CYS C	68	12.794	45.898	39.512	1.00	193.02
30	514 515	CA	CYS C	68	11.523	46.307	40.083	1.00	193.02
30	516	C O	CYS C CYS C	68	11.724	47.110	41.369	1.00	193.02
	517	СВ	CYS C	68 68	12.709 10.604	46.929	42.091	1.00	193.02
	518	SG	CYS C	68	11.079	45.104 43.935	40.336	1.00	142.23
	519	N	GLN C	69	10.780	48.008	41.620 41.636	1.00	142.23
35	520	CA	GLN C	69	10.806	48.882	42.802	1.00 1.00	226.79 226.79
	521	CB	GLN C	69	11.511	50.191	42.437	1.00	248.82
	522	CG	GLN C	69	11.193	51.363	43.344	1.00	248.82
	523	CD	GLN C	69	11.804	52.664	42.851	1.00	248.82
40	524	OE1	GLN C	69	11.623	53.050	41.694	1.00	248.82
40	525 526	NE2 C	GLN C	69	12.526	53.352	43.730	1.00	248.82
	527	ŏ	GLN C GLN C	69	9.370	49.163	43.221	1.00	226.79
	528	Ň	HIS C	69 70	8.470 9.149	49.208 49.349	42.382	1.00	226.79
	529	CA	HIS C	70	7.806	49.635	44.515 45.003	1.00	241.71
45	530	СВ	HIS C	70	7.524	48.852	46.292	1.00 1.00	241.71
	531	CG	HIS C	70	7.366	47.378	46.075	1.00	246.85 246.85
	532	CD2	HIS C	70	7.971	46.319	46.666	1.00	246.85
	533	ND1	HIS C	70	6.487	46.852	45.155	1.00	246.85
50	534	CE1	HIS C	70	u 56	45.530	45.184	1.00	246.85
50	535 536	NE2	HIS C	70	7.448	45.184	46.094	1.00	246.85
	537	C	HIS C HIS C	70	7.601	51.127	45.236	1.00	241.71
	538	Ñ		70 71	8.435	51.946	44.851	1.00	241.71
	539	ČA	GLN C	71 71	6.485 6.139	51.470	45.872	1.00	248.91
55	540	CB	GLN C	71	4.804	52.861 52.897	46.161	1.00	248.91
	541	CG	GLN C	71	4.049	54.235	46.935 46.919	1.00 1.00	249.69
	542	CD	GLN C	71	3.630	54.682	45.519	1.00	249.69 249.69
	543	OE1	GLN C	7 1	3.071	53.904	44.741	1.00	249.69
60	544	NE2	GLN C	71	3.889	55.949	45.201	1.00	249.69
60	545	Ç	GLN C	71	7.243	53.579	46.956	1.00	248.91
	546 547	0	GLN C	71	7.670	54.680	46.599	1.00	248.91
	547 548	N CA	GLN C	72	7.705	52.942	48.026	1.00	236.85
	549	CA CB	GLN C GLN C	72 72	8.741	53.519	48.875	1.00	236.85
65	550	CG	GLN C	72 72	8.117	53.962	50.201	1.00	249.69
	551	CD	GLN C	72	9.064 8.391	54.624 54.885	51.198	1.00	249.69
	552	OE1	GLN C	72	7.360	54.885 55.560	52.545 52.617	1.00	249.69
	553	NE2	GLN C	72	8.973	54.348	52.617 53.617	1.00 1.00	249.69
70	554	Ç	GLN C	72	9.860	52.501	49.127	1.00	249.69 236.85
70	555	0	GLN C	72	10.188	52.188	50.274	1.00	236.85
								-	

								1.00	249.69
			VAL C	73°	10.435	51.975	48.050		249.69
	556	N			11.519	51.001	48.163	1.00	
	557	CA	77.4		11.016	49,546	47.988	1.00	190.27
	558	CB	4 		12.100	48.583	48.424	1.00	190.27
	559	CG1	****		9.740	49,315	48.789	.1.00	190.27
	560	CG2		73		51.280	47.077	1.00	249.69
5	561	C	****		12.547	51.0/4	45.966	1.00	249.69
		Ö			12.195	51.080	47.397	1.00	225.53
	562	Ň	ASN C	74	13.819	51.314	46.426	1.00	225.53
	563	ČA	ASN C	74	14.877	51.480	47.153	1.00	240.44
••	564	CB	ASN C	74	16.220		48.221	1.00	240.44
10	565	CG	ASN C	74	16.174	52.577	47.999	1.00	240.44
	566		ASN C	74	15.597	53.643	49.374	1.00	240.44
	567	OD1	ASN C	74	16.786	52.316		1.00	225.53
	568	ND2	ASN C	74	14.929	50.162	45.407	1.00	225.53
	569	Ç	ASN C	74	14.963	48.987	45.778	1.00	249.69
15	570	0	GLU C	75	14.918	50.516	44.123	1.00	249.69
	571	N	GFO C	75	14.943	49.543	43.030		249.60
	572	ÇA	GLU C	75	15.262	50.260	41.708	1.00	249.60
	573	CB	GLU C GLU C	75	16.260	514	41.834	1.00	249.60
	574	CG			16.362	52.238	40.567	1.00	
20	575	CD	GLU C	7 5	15.308	52.660	40.046	1.00	249.60
20	576	OE1	GLU C	75	17.493	52.480	40.096	1.00	249.60
	577	OE2	GLU C	75		48.356	43.233	1.00	249.69
	578	С	GLU C	75	15.886	48.508	43.733	1.00	249.69
	579	0	GLU C	75	16.998	47.175	42.830	1.00	230.56
25	580	N	SER C	76	15.421	45.932	42,968	1.00	230.56
25	581	CA	SER C	76	16.178	44.734	42.596	1.00	187.63
		CB	SER C	76	15.307		41.190	1.00	187.63
	582	ÕĞ	SER C	76	15.123	44.661	42.115	1.00	230.56
	583	c	SER C	76	17.435	45.877	41.124	1.00	230.56
20	584	ŏ	SER C	76	17.565	46.600	42.510	1.00	249.20
30	585	N	GLU C	77	18.356	45.002	41.778	1.00	249.20
	586		GLU C	77	19.602	44.825	42.527	1.00	249.69
	587	CA	GLU C	77	20.531	43.861	43.870	1.00	249.69
	588	CB	GLU C	77	21.030	44.390		1.00	249.69
	589	CG	GLU C	77	21,895	45.639	43.734	1.00	249.69
35	590	CD	GLU C	77	22.002	46.187	42.611	1.00	249.69
	591	OE1	GLU C	77	22.468	46.078	44.755		249.20
	592	OE2	GLU C	77	19.257	44.256	40.410	1.00	249.20
	593	C	GLU C	77	18.786	43.124	40.304	1.00	211.01
	594	0		78	19.492	45.042	39.346	1.00	171.69
40	595	N	PRO C	78	20.275	46.292	39.342	1.00	211.01
	596	CD	PRO C	78 78	19.193	44.608	37.977	1.00	
	597	CA	PRO C		20.023	45.581	37.127	1.00	171.69
	598	CB	PRO C	78	20.054	46.826	37.951	1.00	171.69
	599	CG	PRO C	78	19.580	43.155	37.720	1.00	211.01
45	600	С	PRO C	78	20.416	42.597	38.420	1.00	211.01
	601	0	PRO C	78	18.950	42.537	36.728	1.00	200.35
	602	N	VAL C	79	19.282	41.166	36.344	1.00	200.35
	603	CA	VAL C	79		40.146	36.754	1.00	129.43
	604	CB	VAL C	79	18.203	38.805	36.090	1.00	129.43
50) 605	CG1	VAL C	79	18.471	39.966	38.259		129.43
٦,	606	CG2	VAL. C	79		41.203	34.835	1.00	200.35
	607	C	VAL C	79		41.902	34.191		200.35
	608	ŏ	VAL C	79			34,262		130.20
		Ň	TYR C	80		40.476	32.817		130.20
_	609	ČA	TYR C	80		40.495	32.410		206.ხა
5		CB	TYR C	80		40.686	30.97		206.89
	611	ČĠ	TYR C		22.046	41.126	30.61		206.89
	612	CD1	TYR C		21.927	42.471	29.29		206.89
	613		TYR C	. 8	22.011	42.880	29.95	-	206.89
	614	CE1	TYR	. 8		40.199			206.89
6	615	CD2	TYR	_		40.598	28.62		206.89
	616	CE2	TYR		0 22.217	41.939	28.29		206.89
	617	CZ	TYR		0 22.299	42.339	26.98		130.20
	618	ÓН	TYR		0 19.928	39.237	32.17		130.20
	619	C	ITH	· •	0 20.195	38.133	32.63		124.74
(65 620	0	TYR (19.172	39.406	31.09		124.74
Ţ,	621	N	LEU	-	18.624		30.39		90.50
	622	CA	LEU				30.2		
	623	CB	LEU		31 17.103 81 16. 47 0		29.4		
	624	CG	LEU	<u> </u>			30.1	22 1.00	90.50
	70 625	CD1	LEU	U I	81 16.710				

	626	CD2		• •	4.994 9.216	37.467 38.222	29.222 28.998	1.00 1.00	90.50 124.74
	627	C			9.210 9.179	39.232	28.300	1.00	124.74
	628	0			9.771	37.075	28.595	1.00	106.68
-	629	N ·		-	0.322	36.967	27.253	1.00	106.68
5	630	CA CB			1.797	36.601	27.305	1.00 1.00	249.60 249.60
	631	CG	GLU C	82 2	2.564	37.080	26.079 26.143	1.00	249.60
	632 633	CD	GLU C		24.041	36.748 36.761	27.257	1.00	249.60
	634	OE1	GLU C		24.609	36.489	25.075	1.00	249.60
10	635	OE2	GLU C		24.637 19.546	35.917	26.454	1.00	106.68
	636	C	GLU C		19.224	34.834	26.994	1.00	106.68
	637	0	VAL C		19.234	36.244	25.186	1.00	145.59 145.59
	638	N CA	VAL C		18.513	35.318	24.292 23.679	1.00 1.00	134.02
15	639 _. 640	CB	VAL C		17.270	35.943	22.796	1.00	134.02
13	641	CG1	VAL C		16.562	34.914 36.429	24.781	1.00	134.02
	642	CG2	VAL C		16.343 19.417	34.835	23.164	1.00	145.59
	643	C	VAL C	83 83	20.212	35.603	22.600	1.00	145.59
	644	0	VAL C PHE C	84	19.259	33.562	22.822	1.00	150.61 150.61
20	645	N CA	PHE C	84	20.117	32.945	21.833	1.00 1.00	134.04
	646	CB	PHE C	84	21.072	31.978	22.515 23.516	1.00	134.04
	647 648	CG	PHE C	84	21.985	32.603 32.852	24.818	1.00	134.04
	649	CD1	PHE C	84	21.566	32.918	23.158	1.00	134.04
25	650	CD2	PHE C	84	23.282 22.433	33.403	25.743	1.00	134.04
	651	CE1	PHE C	84 84	24,151	33.468	24.078	1.00	134.04
	652	CE2	PHE C PHE C	84	23.729	33.712	25.370	1.00	134.04 150.61
	653	CZ C	PHE C	84	19.487	32.151	20.719	1.00 1.00	150.61
. 20	654	Ö	PHE C	84	18.363	31.654	20.842 19.653	1.00	176.12
30	655 656	Ň	SER C	85	20.276	31.999 31.208	18.491	1.00	178.12
	657	CA	SER C	85	19.898	32.073	17.269	1.00	141.64
	658	CB	SER C	85 es	19.635 19.275	31.250	16.175	1.00	141.64
	659	og.	SER C SER C	85 85	21.092	30.334	18.214	1.00	176.12
35	660	C	SER C	85	22.171	30.838	17.876	1.00 1.00	176.12 126.17
	661	0 N	ASP C	86	20.900	29.030	18.377 18.156	1.00	126.17
	662 663	CA	ASP C	86	21.976	28.062	19.122	1.00	148.28
	664	СВ	ASP C	86	23.135	28.325 28.085	18.490	1.00	148.28
40	665	CG	ASP C	86	24.477 24.674	26.995	17.898	1.00	148.28
	666	OD1	ASP C	86 86	25.329	28.999	18.587	1.00	148.28 126.17
	667	OD2	ASP C ASP C	86	21.448	26.656	18.392	1.00	126.17
	668	CO	ASP C	86	20.356	26.480	18.922 18.003	1.00 >- 1.00	154.85
45	669 670	Ň	TRP C	87	22,220	25.650 24.277	18.204	1.00	154.85
43	671	CA	TRP C	87	21.780	23.312	17.473	1.00	249.47
	672	CB	TRP C	87 97	22.714 22.275	23.058	16.067	1.00	249.47
	673	CG	TRP C	87 87	22.713	23.754	14.895	1.00	249.47
	674	CD2	TRP C	87	22.000	23.217	13.798	1.00	249.47 249.47
50		CE2 CE3	TRP C	87	23.645	24.782	14.661 15.650	1.00 1.00	249.47
	676 677	CD1	TRP C	87	21.335	22.152 22.243	14.290		249.47
	678	NE1	TRP C	87	21.165	23.670	12.489		249.47
	679	CZ2	TRP C	87 97	22.184 23.828	25.232	13.361	1.00	249.47
5	5 680	CZ3	TRP C	87 87	23.098	24.675	12.291		249.47 154.85
	681	CH2	TRP C	87	21.715	23.947	19.683		154.85
	682 683	C	TRP C	87	20.676	23.513	20.170 20.394		160.72
	684	Ň	LEU C		22.820	24.160 23.888	21.82		160.72
6	0 685	CA	LEU C		22.851	22,726	22.12		161.67
·	686	CB	LEU C		23.811 23.421	21.360	21.54		161.67
	687	CG	LEU C		24.392	20.299	22.02		161.67
	688	CD1	LEU C		22.005	21.001	21.96		161.67 160.72
	689	CD2 C	LEU	; 88		25.124	22.62		160.72
C	690	ŏ	LEU	; 88	24.103	25.909	22.19 23.78		139.08
	691 692	Ň	LEU C	89		25.306 26.426	24.65		139.08
	693	CA	LEU			27.440	24.66	3 1.00	166.24
	694	CB	LEU (25.62		166.24
· ·	70 695	CG	LEU	, ,,					

	696	CD1	LEU C	89	23.405	29.250	25.356	1.00	166.04
	697	CD2	LEU C	89	20.917	29.623	25.492	1.00	166.24 166.24
	698	C .	LEU C	89	23.123	25.891	26.057	1.00	139.08
5	699 700	N .	LEU C	89	22.297	25.098	26.533	1.00	139.08
,	701	CA	LEU C	90 90	24.212 24.490	26.304 25.844	26.715	1.00	149.33
	702	CB	LEU C	90	25.993	25.806	28.077 28.323	1.00 1.00	149.33
	703	CG	LEU C	90	26.370	25.474	29.765	1.00	143.04 143.04
10	704	CD1	LEU C	90	25.808	24.104	30.144	1.00	143.04
10	705 706	CD2 C	LEU C	90	27.884	25.509	29.938	1.00	143.04
	707	ŏ	LEU C	90 90	23.834 24.213	26.755 27.914	29.106	1.00	149.33
	708	Ň	GLN C	91	22.861	26.226	29.243 29.839	1.00 1.00	149.33
	709	CA	GLN C	91	22.166	27.026	30.825	1.00	125.14 125.14
15	710	СВ	GLN C	91	20.656	26.784	30.745	1.00	164.13
	711 712	CG	GLN C	91	20.043	27.113	29.398	1.00	164.13
	712	CD OE1	GLN C GLN C	91	18.552	26.873	29.373	1.00	164.13
	714	NE2	GLN C	91 91	18.078 17.799	25.769 27.910	29.661	1.00	164.13
20	715	C	GLN C	91	22.633	26.746	29.035 32.238	1.00 1.00	164.13
	716	0	GLN C	91	22.832	25.583	32.625	1.00	125.14 125.14
	717	N	ALA C	92	22.787	27.820	33.014	1.00	120.03
	718	CA	ALA C	92	23.217	27.706	34.404	1.00	120.03
25	719 720	CB C	ALA C ALA C	92	24.586	28.363	34.567	1.00	230.41
25	720 721	Ö	ALA C ALA C	92 92	22.204 21.618	28.360	35.331	1.00	120.03
	722	Ň	SER C	93	22.009	29.392 27.738	34.993 36.490	1.00	120.03
	723	CA	SER C	93	21.091	28.244	37.499	1.00 1.00	162.82 162.82
-	724	СВ	SER C	93	21.158	27.396	38.784	1.00	102.92
30	725	OG.	SER C	93	22.476	27.269	39.270	1.00	102.92
	726	C	SER C	93	21.472	29.682	37.798	1.00	162.82
	727 728	0 N	SER C ALA C	93	20.699	30.618	37.567	1.00	162.82
	729	CA	ALA C	94 94	22.679 23.224	29.849 31.174	38.313	1.00	108.42
35	730	СВ	ALA C	94	23.252	31.403	38.620 40.121	1.00 1.00	108.42 218.96
	731	C	ALA C	94	24.643	31.150	38.051	1.00	108.42
	732	0	ALA C	94	25.237	30.083	37.932	1.00	108.42
	733	N	GLU C	95	25.180	32.303	37.678	1.00	153.28
40	734 735	CA CB	GLU C	95	26.518	32.317	37.122	1.00	153.28
10	736	CG	GLU C	95 95	26.615 25.708	33.364 33.060	36.025	1.00	202,07
	737	CD	GLU C	95	25.982	33.949	34.858 33.677	1.00 1.00	202.07
	738	OE1	GLU C	95	25.257	33.821	32.668	1.00	202.07 202.07
15	739	OE2	GLU C	95	26.925	34.772	33.751	1.00	202.07
45	740	C	GLU C	95	27.586	32.559	38.176	1.00	153.28
	741 742	0 N	GLU C VAL C	95	28.757	32.209	37.973	1.00	153.28
	743	GA	VAL C	96 96	27.180 28.105	33.151 33.428	39.302	1.00	129.17
	744	CB	VAL C.	96	28.289	34.930	40.407 40.613	1.00 1.00	129.17
50	745	CG1	VAL C	96	29.526	35.175	41.441	1.00	121.01 121.01
	746	CG2	VAL C	96	28.379	35.630	39.273	1.00	121.01
	747	C	VAL C	96	27.548	32.826	41.694	1.00	129.17
	748 749	O N	VAL C	96	26.380	33.012	42.009	1.00	129.17
55	750	CA CA	VAL C VAL C	97 97	28.383 27.885	32.123	42.449	1.00	144.84
	751	CB	VAL C	97	27.555 27.554	31.495 30.011	43.658 43.391	1.00	144.84
	752	CG1	VAL C	97	26.631	29.492	44.443	1.00 1.00	123.55 123.55
	753	CG2	VAL C	97	27.013	29.816	42.007	1.00	123.55
60	754	C	VAL C	97	28.756	31.574	44.921	1.00	144.84
00	755 756	0 N	VAL C	97	29.987	31.649	44.847	1.00	144.84
	757	CA	MET C MET C	98 98	28.083 28.713	31.537	46.073	1.00	143.10
	758	CB	MET C	98	27.725	31.568 32.094	47.396	1.00	143.10
	759	CG	MET C	98	27.725 27.288	33.530	48.440 48.256	1.00 1.00	249.69 249.69
65	760	SD	MET C	98	28.558	34.688	48.776	1.00	249.69
	761	CE	MET C	98	28.400	34.595	50.561	1.00	249.69
	762	C	MET C	98	29.093	30.140	47.792	1.00	143.10
	763 764	0 N	MET C	98	28.224	29.260	47.820	1.00	143.10
70	765	CA	GLU C	99 99	30.366 30.817	29.905	48.115	1.00	134.64
-				93	00.017	28.560	48.495	1.00	134.64

	766	СВ	GLU C	99	32.113	28.640	49.296	1.00	242.00
	767	CG	GLU C	99	32.954	27.373	49.225	1.00 1.00	249.69
	768	CD:	GLU C	99	34.077	27.361	50.242	1.00	249.69
_	769	OE1	GLU C	99	34.676	28.433	50.488	1.00	249.69
5	770	OE2	GLU C	99	34.370	26.275	50.787	1.00	249.69 249.69
	771	С	GLU C	99	29.760	27.848	49.328	1.00	134.64
	772	0	GLU C	99	29.307	28.382	50.333	1.00	134.64
	773	N	GLY C	100	29.348	26.660	48.899	1.00	174.64
10	774	ÇA	GLY C	100	28.349	25.925	49.654	1.00	174.64
10	775	C	GLY C	100	26.950	25.885	49.070	1.00	174.64
	776	0	GLY C	100	26.164	25.012	49.424	1.00	174.64
	777	N	GLN C	101	26.630	26.825	48.185	1.00	145.91
	778 779	CA	GLN C	101	25.309	26.876	47.562	1.00	145.91
15	779 780	CB	GLN C	101	25.060	28.258	46.9 6 0	1.00	202.42
15	781	CG CD	GLN C GLN C	101	24.842	29.331	47.995	1.00	202.42
	782	OE1	GLN C GLN C	101	23.913	28.865	49.091	1.00	202.42
	783	NE2	GLN C	101 101	24.266	27.997	49.893	1.00	202.42
	784	C	GLN C	101	22.712 25.106	29.428 25.805	49.123	1.00	202.42
20	785	ŏ	GLN C	101	26.031	25.0 6 3	46.487	1.00	145.91
	786	Ň	PRO C	102	23.886	25.701	46.149 45.030	1.00	145.91
	787	CD	PRO C	102	22.626	26.310	45.939 46.410	1.00	126.29
	788	CA	PRO C	102	23.621	24.698	44.908	1.00	226.98
	789	СВ	PRO C	102	22.151	24.385	45.124	1.00 1.00	126.29
25	790	CG	PRO C	102	21.598	25.737	45.443	1.00	226.98 226.98
	791	С	PRO C	102	23.911	25.213	43.497	1.00	126.29
	792	0	PRO C	102	23.787	26.412	43.199	1.00	126.29
	793	N	LEU C	103	24.286	24.291	42.620	1.00	131.06
20	794	CA	LEU C	103	24.592	24.644	41.240	1.00	131.06
30	795	CB	LEU C	103	26.086	24.692	41.058	1.00	130.31
	796	CG	LEU C	103	26.385	25.294	39.703	1.00	130.31
	797	CD1	LEU C	103	25.983	26.756	39.788	1.00	130.31
	798 799	CD2	LEU C	103	27.857	25.143	39.332	1.00	130.31
35	800	C	LEU C	103 103	24.020	23.658	40.214	1.00	131.06
	801	Ň	PHE C	104	24.265 23.267	22.458	40.297	1.00	131.06
	802	CA	PHE C	104	22.698	24.151 23.265	39.239 38.229	1.00	115.91
	803	CB	PHE C	104	21.177	23.174	38.354	1.00 1.00	115.91
	804	CG	PHE C	104	20.701	22.781	39.706	1.00	184.63 184.63
40	805	CD1	PHE C	104	20.673	23.704	40.748	1.00	184.63
	806	CD2	PHE C	104	20.284	21.483	39.950	1.00	184.63
	807	CE1	PHE C	104	20.232	23.335	42.025	1.00	184.63
:	808	CE2	PHE C	104	19.841	21.104	41.225	1.00	184.63
45	809 810	CZ	PHE C	104	19.815	22.034	42.264	1.00	184.63
43	811	C	PHE C	104	23.026	23.754	36.826	1.00	115.91
	812	N	PHE C LEU C	104 105	22.731	24.898	36.464	1.00	115.91
	813	ČA	LEU C	105	23.636 23.955	22.890	36.025	1.00	135.47
	814	CB	LEU C	105	25.417	23.247 23.009	34.643	1.00	135.47
50	815	ČĠ	LEU C	105	26.347	23.800	34.331	1.00	111.96
	816	CD1	LEU C	105	27.796	23.589	35.242 34.767	1.00 1.00	111.96
	817	CD2	LEU C	105	25.961	25.269	35.233	1.00	111.96
	818	C	LEU C	105	23.101	22.381	33.740	1.00	111.96 135.47
	819	0	LEU C	105	22.734	21.264	34.094	1.00	135.47
55	820	N	ARG U	106	22.782	22.888	32.564	1.00	142.54
	821	CA	ARG C	106	21.928	22.134	31.679	1.00	142.54
	822	CB	ARG C	106	20.500	22.619	31.876	1.00	187.32
	823	ca	ARG C	106	19.479	21.927	31.044	1.00	187.32
60	824 825	CD	ARG C	106	18.129	22.598	31.190	1.00	187.32
00	826	NE CZ	ARG C	106	17.177	22.007	30.262	1.00	187.32
	827	NH1	ARG C	106	16.158	22.658	29.719	1.00	187.32
	828	NH2	ARG C	106	15.956	23.937	30.020	1.00	187.32
	829	C	ARG C ARG C	106	15.359	22.032	28.858	1.00	187.32
65	830	ŏ	ARG C	106 106	22.347 22.485	22.297	30.232	1.00	142.54
_	831	Ň	CYS C	107	22.465 22.580	23.424 21.177	29.750 20.547	1.00	142.54
	832	CA	CYS C	107	22.950	21.177 21.221	29.547	1.00	145.66
	833	C	CYS C	107	21.612	21.282	28.129 27.439	1.00 1.00	145.66
70	834	0	CYS C	107	20.923	20.257	27.350	1.00	145.66 145.66
70	835	CB	CYS C	107	23.679	19.945	27.717	1.00	147.17
									177.17

	836	sg N			1.521 1.242	20.003 22.477	26.086 26.975	1.00 1.00	147.17 187.51
	837 838	CA			9.945	22.697	26.334	1.00	187.51 249.50
	839	CB .			9.369	24.051	26.763 26.389	1.00 1.00	249.50
5	840	CG	HIS C		7.934	24.251 25.271	25.756	1.00	249.50
•	841	CD2	HIS C		7.311 6.945	23.348	26.724	1.00	249.50
	842	ND1	HIS C HIS C		5. 777	23.808	26.317	1.00	249.50
	843	CE1	HIS C HIS C		5.969	24.974	25.727	1.00	249.50
10	844	NE2 C	HIS C		9.929	22.622	24.824	1.00	187.51
10	845 846	ŏ	HIS C	108 2	0.677	23.334	24.148	1.00 1.00	187.51 207.18
	847	Ň	GLY C		9.049	21.765 21.601	24.310 22.879	1.00	207.18
	848	CA	GLY C		8.916	22.668	22.337	1.00	207.18
	849	Ç	GLY C		7.989 7.304	23.341	23.106	1.00	207.18
15	850	0	GLY C TRP C		7.976	22.837	21.017	1.00	133.19
	851	N CA	TRP C		7.119	23.828	20.384	1.00	133.19
	852 853	CB	TRP C		17.724	24.269	19.044	1.00 1.00	164.64 164.64
	854	ČĠ	TRP C		16.806	25.128	18.221 18.110	1.00	164.64
20	855	CD2	TRP C		16.829	26.561 26.928	17.286	1.00	164.64
	856	CE2	TRP C		15.742 17.659	27.566	18.625	1.00	164.64
	857	CE3	TRP C		15.753	24.710	17.479	1.00	164.64
	858	CD1	TRP C		15.103	25.780	16.917	1.00	164.64
25	859	NE1 CZ2	TRP C		15.460	28.261	16.964	1.00	164.64 164.64
25	860 861	CZ3	TRP C	110	17.380	28.901	18.301 17.474	1.00 1.00	164.64
	862	CH2	TRP C		16.285	29.231	20.194	1.00	133.19
	863	С	TRP C	110	15.711	23.243 22.018	20.064	1.00	133.19
	864	0	TRP C	110	15.535 14.709	24.124	20.194	1.00	142.65
30	865	N	ARG C ARG C	111 111	13.309	23.711	20.051	1.00	142.65
	866	CA	ARG C	111	13.020	23.259	18,618	1.00	249.69
	867	CB CG	ARG C	111	12.569	24.383	17.699	1.00 1.00	249.69 249.69
	868 869	CD	ARG C	111	11.976	23.832	16.409 16.004	1.00	249.69
35	870	NE	ARG C	111	10.799	24.593 24.725	16.755	1.00	249.69
55	871	CZ	ARG C	111	9.704 9.634	24.144	17.952	1.00	249.69
	872	NH1	ARG C ARG C	111 111	8.674	25.440	16.311	1.00	249.69
	873	NH2	ARG C	111	12.979	22.588	21.013	1.00	142.65 142.65
40	874	CO	ARG C	111	12.125	21.759	20.747	1.00 1.00	230.43
40	875 876	Ň	ASN C	112	13.675	22.582	22.137 23.156	1.00	230.43
	877	CA	ASN C	112	13.477	21.574 21.797	23.858	1.00	249.69
	878	СВ	ASN C	112	12.133 12.030	21.045	25.178	1.00	249.69
	879	CG	ASN C ASN C	112 112	12.829	20.147	25.466	1.00	249.69
45	880	OD1 ND2	ASN C ASN C	112	11.036	21.404	25.983	1.00	249.69 230.43
	881	C	ASN C	112	13.531	20.163	22.573	1.00 1.00	230.43
	882 883	ŏ	ASN C	112	12.862	19.257	23.075 21.511	1.00	206.47
	884	N	TRP C	1 4	14.310	19.970 18.637	20.916	1.00	206.47
50	885	CA	TRP C	113	14.426 15.220	18.665	19.611	1.00	233.56
	886	CB	TRP C	113 113	14.430	19.060	18.428	1.00	233.56
	887	CG CD2	TRP C	113	14.905	19.800	17.309	1.00	233.56 233.56
	888 889	CE2	TRP C	113	13.832	19.895	16.392	1.00 1.00	233.56
55	890	CE3	TRP C	113	16.129	20.395	16.990 18.158	1.00	233.56
5.	891	CD1	TRP C	113	13.132	18.740 19.239	16.937	1.00	233.56
	892	NE1	TRP C	113	12.764 13.952	20.566	15.166		233.56
	893	CZ2	TRP C	113 113	16.253	21,061	15.772		233.56
-	894	CZ3 CH2	TRP C	113	15,165	21.139	14.873		233.56 206.47
60) 895 896	C	TRP C	113	15.137	17.714	21.887		206.47
	897	· ŏ	TRP C	113	15.328	18.062	23.050 21.408		249.46
	898	N	ASP C	114	15.535	16.540	22.256		249.46
	899	CA	ASP C	114		15.589 14.218	22.229		249.69
6		CB	ASP C	114 114		14.137	23.189	1.00	249.69
	901	CG	ASP C			14.363	24.407		249.69
	902	OD1 OD2	. ASP C			13.838	22.729		249.69 249.46
	903 904	C	ASP C	: 114	17.704	15.447	21.83- 20.64		249.46
7	0 905	ŏ	ASP C	; 114	18.008	15.291	20.04		
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	906	N	VAL C	115	18.602	15.512	22.818	1.00	150.51
	907	CA	VAL C	115	20.027	15.388	22.545	1.00	150.51
	908 909	CB CG1 ·	VAL C VAL C	115 115	20.831 22.243	16.572	23.147	1.00	133.46
5	910	CG2	VAL C	115	20.140	16.592 17.884	22.569 22.859	1.00 1.00	133.46
	911	С	VAL C	115	20.559	14.078	23.135	1.00	133.46 150.51
	912	0	VAL C	115	20.153	13.669	24.225	1.00	150.51
	913 914	N CA	TYR C TYR C	116 116	21.468	13.432	22.404	1.00	198.57
10	915	CB	TYR C	116	22.066 21.673	12.170 11.070	22.826 21.847	1.00 1.00	198.57
	916	CG	TYR C	116	20.185	10.787	21.832	1.00	249.69 249.69
	917	CD1	TYR C	116	19.350	11.339	20.856	1.00	249.69
	918 919	CE1 CD2	TYR C TYR C	116	17.974 19.608	11.099	20.866	1.00	249.69
15	920	CE2	TYR C	116 116	18.241	9.987 9.741	22.816 22.838	1.00 1.00	249.69
	921	CZ	TYR C	116	17.429	10.296	21.865	1.00	249.69 249.69
	922	ОH	TYR C	116	16.075	10.047	21.894	1.00	249.69
	923 924	C O	TYR C TYR C	116	23.582	12.257	22.914	1.00	198.57
20	925	Ň	LYS C	116 117	24.174 24.198	13.239 11.230	22.455 23.500	1.00	198.57
	926	CA	LYS C	117	25.660	11.186	23.661	1.00 1.00	159.55 159.55
	927	CB	LYS C	117	26.357	10.893	22.320	1.00	249.69
	928 929	CG CD	LYS C	117	26.455	9.408	21.969	1.00	249.69
25	930	CE	LYS C	117 117	27.543 28.915	9.165 9.642	20.910	1.00	249.69
	931	NZ	LYS C	117	30.027	9.430	21.399 20.424	1.00 1.00	249.69 249.69
	932	C	LYS C	117	26.242	12.486	24.245	1.00	159.55
	933 934	O N	LYS C	117	27.200	13.081	23.698	1.00	159.55
30	935	CA	VAL C VAL C	118 118	25.675 26.095	12.904 14.127	25.371	1.00	141.55
	936	CB	VAL C	118	24.919	14.737	26.016 26.790	1.00 1.00	141.55 150.57
	937	CG1	VAL C	118	25.416	15.626	27.908	1.00	150.57
	938 939	CG2 C	VAL C	118	24.067	15.543	25.830	1.00	150.57
35	940	ŏ	VAL C VAL C	118 118	27.305 27.466	14.028 13.067	26.927	1.00	141.55
	941	Ň	ILE C	119	28.140	15.062	27.672 26.850	1.00 1.00	141.55 119.98
	942	CA	ILE C	119	29.358	15.192	27.640	1.00	119.98
	943 944	CB CG2	ILE C	119	30.578	14.818	26.826	1.00	122.95
40	945	CG1	ILE C	119 119	31.814 30.368	14.861 13.438	27.700	1.00	122.95
	946	CD1	ILE C	119	31.187	13.436	26.214 24.988	1.00 1.00	122.95 122.95
	947	Ç	ILE C	119	29.528	16.649	28.029	1.00	119.98
	948 949	0 N	ILE C	119	29.454	17.518	27.179	1.00	119.98
45	950	CA	TYR C TYR C	120 120	29.744 29.962	16.919 18.289	29.310	1.00	136.43
	951	CB	TYR C	120	29.334	18.542	29.759 31.119	1.00 1.00	136.43 134.07
	952	CG	TYR C	120	27.833	18.525	31.107	1.00	134.07
	953 954	CD1 CE1	TYR C	120	27.125	17.332	31.234	1.00	134.07
50	955	CD2	TYR C TYR C	120 120	25.733 27.113	17.310 19.704	31.200	1.00	134.07
	956	CE2	TYR C	120	25.721	19.705	30.949 30.912	1.00 1.00	134.07 134.07
	957	CZ	TYR C	120	25.037	18.507	31.037	1.00	134.07
	958 959	о́н	TYR C	120	23.658	18.523	30.988	1.00	134.07
55	960	CO	TYR C TYR C	120 120	31.455 32.171	18.459 17.497	29.877	1.00	136.43
	961	Ň	TYR C	121	31.935	19.674	30.131 29.682	1.00 1.00	136.43
	962	CA	TYR C	121	33.366	19.916	29.782	1.00	132.15 132.15
	963 964	CB	TYR C	121	33.991	20.177	28.405	1.00	142.37
60	965	CG CD1	TYR C TYR C	121 121	34.032 32.863	19.017 18.383	27.437	1.00	142.37
	966	CE1	TYR C	121	32.889	17.388	27.007 26.038	1.00 1.00	142.37 142.37
	967	CD2	TYR C	121	35.237	18.620	26.879	1.00	142.37
	968	CE2	TYR C	121	35.284	17.616	25.900	1.00	142.37
65	969 970	CZ OH	TYR C TYR C	121 121	34.098 34.141	17.005	25.481	1.00	142.37
	971	Č.	TYR C	121	33.668	16.024 21.119	24.499 30.667	1.00 1.00	142.37
	972	0	TYR C	121	33.025	22.159	30.543	1.00	132.15 132.15
	973 974	N	LYS C	122	34.650	20.977	31.554	1.00	126.92
70	975	CA CB	LYS C LYS C	122 122	35.056 34.793	22.076 21.754	32.413	1.00	126.92
_		~ ~			J7./ 33	21.754	33.878	1.00	206.28

	976	CG		122 35.177 122 35.209	22.888 22.4 2 0	36.238	1.00 1.00	206.28 206.28
	977	CD CE		122 35.768	23.480		1.00	206.28 206.28
	978	NZ .		122 35.923	22.930		1.00 1.00	126.92
5	979 980	C		122 36.544	22.299		1.00	126.92
5	981	ŏ	LYS C	122 37.349	21.420 23.477	31.699	1.00	135.65
	982	N		123 36.902 123 38.294	23.827	31.435	1.00	135.65
	983	CA		123 38.294 123 39.093	23.949	32,740	1.00	170.94
	984	CB	ASP C ASP C	123 38.763	25.212	33.507	1.00	170.94
10	985	CG OD1	ASP C	123 38.780	26.308	32.904	1.00	170.94 170.94
	986	OD2	ASP C	123 38.496	25.117	34.721 30.509	1.00 1.00	135.65
	987 988	C	ASP C	123 38.987	22.847	30.818	1.00	135.65
	989	ŏ	ASP C	123 40.082	22.372 22.547	29.378	1.00	178.68
15	990	N	GLY C	124 38.345 124 38.917	21.638	28.395	1.00	178.68
	991	ÇA	GLY C	124 38.917 124 38.936	20.152	28.718	1.00	178.68
	992	C	GLY C	124 39.295	19.336	27.879	1.00	178.68 128.18
	993	0 N	GLU C	125 38.539	19.797	29.929	1.00 1.00	128.18
20	994 995	CA	GLU C	125 38.536	18.407	30.368 31.847	1.00	249.69
20	996	СВ	GLU C	125 38.963	18.324 18.660	32,115	1.00	249.69
	997	CG	GLU C	125 40.422	17.552	31.693	1.00	249.69
	998	CD	GLU C	125 41.355 125 41.251	16.453	32.273	1.00	249.69
	999	OE1	GLU C	125 42.189	17.777	30.786	1.00	249.69
25	1000	OE2 · · ·	GLU C	125 37.176	17.749	30.215	1.00 1.00	128.18 128.18
	1001	ŏ	GLU C	125 36.149	18.395	30.403 29.866	1.00	114.67
	1002 1003	Ň	ALA C	126 37.165	16.468	29.753	1.00	114.67
	1004	CA	ALA C	126 35.904	15.742 14.376	29.162	1.00	125.78
30	1005	СВ	ALA C	126 36.156 126 35.397	15.622	31.195	1.00	114.67
	1006	C	ALA C ALA C	126 35.397 126 36.190	15.374	32.099	1.00	114.67
	1007	0 N	LEU C	127 34.101	15.788	31.437	1.00 1.00	138.95 136.95
	1008 1009	CA	LEU C	127 33.633	15.718	32.816 33.235	1.00	112.43
35	1010	СВ	LEU C	127 33.090	17.062 17.216	34.734	1.00	112.43
33	1011	CG	LEU C	127 33.259 127 34.725	17.020	35.093	1.00	112.43
	1012	CD1	LEU C	127 34.725 127 32.768	18.588	35.170	1.00	112.43
	1013	CD2	LEU C	127 32.612	14.648	33.156	1.00	136.95 136.95
40	1014	C	LEU C	127 32.870	13.803	34.019	1.00 1.00	111.10
40	1015 1016	N	LYS C	128 31.444	14.696	32.518 32.750	1.00	111.10
	1017	CA	LYS C	128 30.397	13.689 14.302	33.525	1.00	196.03
	1018	CB	LYS C	128 29.228 128 29.586	14.833	34.905	1.00	196.03
	1019	ca	LYS C Lys C	128 29.586 128 29.864	13.714	35.892	1.00	196.03
45		CD CE	LYS C	128 30.150	14.277	37.285	1.00	196.03 196.03
	1021	NZ	LYS C	128 30.192	13.214	38.329 31.379	1.00 1.00	111.10
	1022 1023	C	L'IS C	128 29.929	13.215	30.360	1.00	111.10
	1024	ŏ	LYS C	128 30.196	13.874 12.078	31.339	1.00	147.54
50) 1025	N	TYR C	129 29.243 129 28.753	11.567	30.058	1.00	147.54
	1026	CA	TYR C	129 29.834	10.755	29.363	1.00	149.35
	1027	CB CG	TYR C	129 29.282	9.856	28.292	1.00 1.00	149.35 149.35
	1028 1029	CD1	TYR C	129 29.066		27.005 26.029	1.00	149.35
5	5 1030	CE1	TYR C	129 28.507		28.584	1.00	149.35
	1031	CD2	ITH C	129 28.929 129 28.371		27.619	1.00	149.35
	1032	CE2	TYR C	129 28.371 129 28.161		26.340	1.00	149.35
	1033	CZ	TYR C TYR C	129 27.613		25.373	1.00	149.35 147.54
-	1034	C OH	TYR C	129 27.500) 10.704	30.177	1.00 1.00	147.54
C	0 1035 1036	ŏ	TYR C	129 27.38		31.098 29.231	1.00	199.38
	1037	Ň	TRP C	130 26.57		29.216		199.38
	1038	CA	TRP C			30.022		218.46
	1039	СВ	TRP C			31.370	1.00	218.46
•	55 1040	CG CD2	TRP C			32.632		218.46 218.46
	1041	CD2 CE2	TRP C		0 11.627	33.631		218.46
	1042 1043	CE3	TRP C	130 23.51	7 9.648	33.029 31.639		218.46
	1043	CD1	TRP C	130 25.32		32.992		218.46
•	70 1045	NE1		130 25.43	12.652	J2.00		

					11.381	34.996	1.00	218.46
1046	CZ2			24.605 23.349	9.398	34.390	1.00	218.46
1047	CZ3			23.895	10.258	35.357	1.00	218.46
1048	CH2			24. 79 4	9.910	27.794	1.00	199.38
1049	C			25 <i>.2</i> 72	10.526	26.839	1.00	199.38
5 1050	0			23.787	9.053	27.671	1.00 1.00	229.56 229.56
1051	N		131	23.148	8.778	26.386	1.00	246.37
1052	CA CB			22.591	7.356	26.372 24.998	1.00	246.37
1053	CG	TYR C		22.180	6.894	24.930	1.00	246.37
1054 10 1055	CD1	TYR C		23.142	6.593	22.748	1.00	246.37
10 1055 1056	CE1	TYR C		22.771	6.206 6.795	24.647	1.00	246.37
1057	CD2	TYR C	131	20.834	6.411	23.370	1.00	246.37
1058	CE2	TYR C	131	20.454 21.422	6.120	22.425	1.00	246.37
1059	CZ	TYR C	131	21.037	5.759	21.152	1.00	246.37
15 1060	OH	TYR C	131 131	22.003	9.783	26.290	1.00	229.56
1061	Č	TYR C TYR C	131	22.194	10.887	25.767	1.00	229.56 249.69
1062	0	GLU C	132	20.814	9.387	26.766	1.00	249.69
1063	N	GLU C	132	19.674	10.303	26.812	1.00 1.00	249.69
1064	CA CB	GLU C	132	18.455	9.632	27.444 26.529	1.00	249.69
20 1065	CG	GLU C	132	17.670	8.696	26.293	1.00	249.69
1066 1067	CD	GLU C	132	16.251	9.186	27.021	1.00	249.69
1068	OE1	GLU C	132	15.815	10.108 8.651	25.388	1.00	249.69
1069	OE2	GLU C	132	15.566	11.278	27.798	1.00	249.69
25 1070	С	GLU C	132	20.299	10.849	28.865	1.00	249.69
1071	0	GLU C	132	20.759 20.318	12.573	27.483	1.00	172.36
1072	N	ASN C	133 133	21.034	13.476	28.374	1.00	172.36
1073	CA	asn c asn c	133	21.319	14.844	27.675	1.00	175.23 175.23
1074	CB	ASN C	133	20.166	15.840	27.735	1.00	175.23
30 1075	CG CD1	ASN C	133	18.999	15.492	27.529	1.00 1.00	175.23
1076	OD1 ND2	ASN C	133	20.506	17.113	27.974 29.815	1.00	172.36
1077	C	ASN C	133	20.565	13.626	30,290	1.00	172.36
1078	ŏ	ASN C	133	19.680	12.906	30.522	1.00	165.75
1079 35 1080	Ň	HIS C	134	21.238	14.521 14.757	31.918	1.00	165.75
1081	CA	HIS C	134	20.960	13.910	32.756	1.00	249.69
1082	CB	HIS C	134	21.912 21.588	13.916	34.223	1.00	249.69
1083	CG	HIS C	134 134	22.305	14.372	35.277	1.00	249.69
1084	CD2	HIS C HIS C	134	20.407	13.441	34.715	1.00	249.69 249.69
40 1085	ND1	HIS C HIS C	134	20.390	13.599	36.041	1.00 1.00	249.69
1086	CE1	HIS C	134	21.526	14.161	36.397	1.00	165.75
1087	NE2 C	HIS C	134	21.166	16.233	32.200 31.285	1.00	165.75
1088	ŏ	HIS C	134		17.050	33,470	1.00	159.28
1089 45 1090	Ň	ASN C	135		16.572 17.948	33.879	1.00	159.28
1090	CA	ASN C	135		18.596	34,178	1.00	249.51
1092	СВ	ASN C	135		18.779	32.923	1.00	249.51
1093	CG	ASN C	(35		19.248	31.903		249.51
1094	OD1	ASN C ASN C	135 135		18.439	32.990		249.51 159.28
50 1095	ND2	ASN C ASN C	135		18.001	35.116		159.28
1096	C	ASN C	135		18.08G	36.253 34.884		134.89
1097	O N	ILE C	130	8 23.692	17.946	35.934		134.89
1098	GA	ILE C	130	6 24.734	17.989	35.31		169.29
1099 55 1100	CB	ILE C	13		18.399 19. 72 3	34.59		169.29
1101	CG2	ILE C			18.510	36.40		169.29
1102	ÇG1	ILE C			18.980	35.88	4 1.00	169.29
1103	CD1	ILE C	: 13 : 13		18.906	37.12		134.89
1104	Ç	ILE C			20.125	37.04		134.89 137.39
60 1105	0	ILE C SER C			18.280	38.23		137.39
1106	N CA	SER C			19.000	39.42		121.23
1107	CA CB	SER C		37 22.367	18.437	39.94 41.22	-	121.23
1108	OG	SER C	10	37 22.076	18.966	40.56		137.39
1109 65 1110	_	SER C) 1	37 24.687	19.025	40.50		137.39
1111	_	SER C	3	37 25.458	18.081 20.113	41.3		121.18
1112				38 24.647	20.113	42.4	78 1.00	121.18
1113				38 25.539 38 26.683	~ 4 000	42.1	09 1.00	97.12
1114	СВ	•	~ .	38 26.683 38 27.385	-4 740	43.3		97.12
70 1115		! ILE (C 1	21.000				
				•				

•						_		41.187	1.00	97.12
			ILE C	138	27.646	20.5 21.4		40.528	1.00	97.12
1	116	· ·	ILE C	138	28.637	21.4 20.8		43.697	1.00	121.18
	1117	00.	ILE C	138	24.814	21.5		43.651	1.00	121.18 175.86
	1118		ILE C	138	24.212 24.890	20.	145	44.796	1.00 1.00	175.86
	1119 1120	Ň	THR C	139 139	24.253	20.	532	46.042 46.929	1.00	224.21
3	1121	CA	THR C	139	24.065		297	47.063	1.00	224.21
	1122	CB	THR C	139	25.324		622	46.298	1.00	224.21
	1123	OG1	THR C	139	23.061		.341 .539	46.745	1.00	175.86
_	1124	CG2 C	THR C	139	25.144		.746	46.654	1.00	175.86 19 6 .19
10	1125	0	THR C	139	24.927	21	.024	47.447	1.00 1.00	196.19
	1126	N	ASN C	140	26.149 27.111	21	.852	48.165	1.00	249.69
	1127 1128	CA	ASN C	140 140	27.710		.053	49.330 50.109	1.00	249.69
	1129	CB	ASN C	140	28.741		1.837	49.523	1.00	249.69
15	1130	CG	ASN C	140	29.656		2.417	51.432	1.00	249.69
	1131	OD1	ASN C	140	28.610		1.845 2.213	47.146	1.00	196.19 196.19
	1132	ND2 C	ASN C	140	28.184		1.327	46.560	1.00	134.37
	1133	ŏ	ASN C	140	28.799 28.400	_	3.507	46.932	1.00 1.00	134.37
20	1134 1135	Ň	ALA C	141	29.383	2	3.954	45.949	1.00	79.03
20	1136	CA	ALA C	141 141	28.834	. 2	25.131	45.148 46.507	1.00	134.37
	1137	CB	ALA C	141		. 2	24.317	47.452	1.00	134.37
	1138	C	ALA C ALA C	141	30.896	•	25.112	45.898	1.00	119.18
	1139	0	THR C	142	31.793	,	23.724 23.954	46.281	1.00	119.18 209.05
25	1140	N GA	THR C	142		,	22.720	46.002	1.00	209.05
	1141	CB	THR C	142		•	21.553	46.578	1.00 1.00	209.05
	1142 1143	0G1	THR C	14: 14:	40		22.907	46.602 45.416	1.00	119.18
	1144	CG2	THR C				25.093	44,356	1.00	119.18
30	1145	C	THR C				25.381	45.865	1.00	145.21
,,,	1146	0	VAL C	14	3 34.75		25.741 26.836	45.096	1.00	145.21 137.97
	1147	N CA	VAL C	: 14			27.672	45.910		137.97
	1148	CB	VAL C				26.915	46.096		137.97
35	1149 1150	CG1	VAL		13 37.53 13 36.5		28.993	45.202 43.879		
33	1151	CG2	VAL		43 36.0		26.287	42.881		145.21
	1152	С	VAL (43 36.1		26.981	43.95	1.00	198.77
	1153	0	GLU		44 36.4		25.040 24.445	42.83	3 1.00	
	1154	N CA	GLU	C 1	44 37.1		23.142	43.24		
40		CB	GLU	C 1	44 37.8		23.312	44.33		- 40 00
	1156	çĞ	GLU	•			22.661	45.62		- 40.00
	1157 1158	CD	GLU	~		251	21.428	45.62 46.63		₀ 249.69
	1159	OE1	GLU	•		293	23.377	41.69		O 198.77
4	5 1160	OE2	GLU	•	144 36.	217	24.179 23.892	40.5	31 1.0	
	1161	C	GLU	Č	1.4.4	.656	24.274	41.9	B9 1.0	00 130.51 00 130.51
	1162	0 N	ASP	C		.912	24.049	40.9		, _ <u> </u>
	1163	CA	ASP	С	170	.904 2.523	23.868	41.5	55 1.0 38 1.0	474 00
	1164 50 1165	CB	ASP	C		2.326	22,490	42.1 41.3		00 171.03
•	1166	CG	ASP	C	145 34	2.478	21.503	41.3		00 171.03
	1167	OD1				2.011	22.392	39.5		00 130.51
	1168	OD2	ASF	Č	145 3	3.863	25.213 25.086	38.	351 1.	.00 130.51 .00 126.39
	1169		ASF	C	1	299	26,342			
	55 1170	41	SEI	3 C	170	4.461 4.505	27.546			.00 126.39 .00 126.60
	1171 1172		SEI	R C	140	35.120	28.723			00 126.60
	1173	~	SE	R C		34.403	29.041			126.39
	1174	, og	s SE	R C R C	146	35.343	27.301		351	1.00 126.39
	60 117	5 C	5E	RC	146	36.478	26.850		.072	1.00 222.43
	117	6 0	GL	Y C	147	34.798	27.614 27.410	35	.846	1.00
	117		a Gl	Y C	• • •	35.550	27.771		,	1.00
	117	۰ ^	. GI	LY C		34.769 33.801	28.520		7,000	1.00 222.43 1.00 128.05
	65 116	۰ -	GI	LY C	147 148	35.187	27.238	3	J. 100	1.00 128.05
	116		TI	HR C	148	34,508	27.506	; 3	2.186 1.201	1.00 134.31
	110	₈₂ C	• •	HR C HR C	148	35.474	28.253	,	0.281	1.00 134.31
	11	B3 C	18 11 1931 T	HR C	148	36.046	27.326 28.94	,	1.973	1.00 134.31
	70 11	· .	G2 T	HR C	148	38.609	20.0	_		
	70 11	85 C			•					

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	1186	С	THR C	148	33.949	26.223	31.538	1.00	128.05
	1187	0	THR C	148	34.679	25.363	31.076	1.00	128.05
	1188	N .	TYR C	149	32.634	26.114	31.517	1.00	106.87
_	1189	CA ·	TYR C	149	31.975	24.945 24.510	30.975 31.905	1.00 1.00	106.87
5	1190	CB CC	TYR C TYR C	149 149	30.819 31.204	24.226	33.336	1.00	100.05 100.05
	1191	CG CD1	TYR C	149	31.489	25.254	34.210	1.00	100.05
	1192 1193	CE1	TYR C	149	31.799	24.992	35.538	1.00	100.05
	1194	CD2	TYR C	149	31.247	22.922	33.816	1.00	100.05
10	1195	CE2	TYR C	149	31.557	22.643	35.125	1.00	100.05
	1196	CZ	TYR C	149	31.829	23.676	35.993	1.00	100.05
	1197	OH	TYR C	149	32.111	23.390	37.325	1.00	100.05
	1198	C	TYR C	149	31.404	25.100	29.567 29.077	1.00 1.00	106.87 106.87
15	1199	0	TYR C TYR C	149	31.228 31.105	26.210 23.953	28.946	1.00	100.87
15	1200	N CA	TYR C	150 150	30.490	23.838	27.614	1.00	107.82
	1201 1202	CB	TYR C	150	31.451	24.307	26.499	1.00	160.56
	1203	CG	TYR C	150	32.523	23.336	26.058	1.00	160.56
	1204	CD1	TYR C	150	32.201	22.195	25.317	1.00	160.56
20	1205	CE1	TYR C	150	33.199	21.307	24.872	1.00	160.56
	1206	CD2	TYR C	150	33.873	23.576	26.351	1.00	160.56
	1207	CE2	TYR C	150	34.880	22.698	25.912	1.00	160.56
	1208	CZ	TYR C	150	34.533 35.507	21.564 20.693	25.169 24.719	1.00 1.00	160.56 160.56
25	1209	OH C	TYR C TYR C	150 150	30.111	22.370	27.462	1.00	107.82
25	1210 1211	ŏ	TYR C	150	30.700	21.521	28.119	1.00	107.82
	1212	Ň	CYS C	151	29.112	22.074	26.641	1.00	88.46
	1213	CA	CYS C	151	28.711	20.694	26.450	1.00	88.46
	1214	C	CYS C	151	28.660	20.293	24.976	1.00	88.46
30	1215	0	CYS C	151	28.585	21.155	24.103	1.00	88.46
	1216	CB	CYS C	151	27.359	20.425	27.087	1.00	149.34
	1217	sa	CYS C THR C	151	25.995	21.380 18.981	26.366 24.715	1.00 1.00	149.34 145.00
	1218	N CA	THR C	152 152	28.711 28.675	18.446	23.358	1.00	145.00
35	1219 1220	CB	THR C	152	30.034	17.838	22.951	1.00	154.69
55	1221	OG1	THR C	152	30.213	16.582	23.614	1.00	154.69
	1222	CG2	THR C	152	31.182	18.762	23.334	1.00	154.69
	1223	С	THR C	152	27.631	17.343	23.278	1.00	145.00
40	1224	0	THR C	152	27.420	16.609	24.240	1.00	145.00
40	1225	N	GLY C	153	26.988	17.213	22.125 21.982	1.00 1.00	161.71 161.71
	1226	CA	GLY C GLY C	153 153	25.980 25.515	16.180 15.979	20.558	1.00	161.71
	1227 1228	C O	GLY C	153	25.830	16.783	19.670	1.00	161.71
	1229	Ň	LYS C	154	24.759	14.905	20.345	1.00	155.18
45	1230	CA	LYS C	154	24.249	14.582	19.022	1.00	155.18
	1231	CB	LYS C	154	24.531	13.110	18.710	1.00	249.69
	1232	CG	LYS C	154	24.159	12.677	17.303	1.00	249.69
	1233	CD	LYS C	154	24.540	11.227	17.071	1.00 1.00	249.69
50	1234	CE	LYS C	154	24.106 24.460	10.749 9.317	15.692 15.459	1.00	249.69 249.69
50	1235 1236	NZ C	LYS C Lys C	154 154	22.748	14.876	18.895	1.00	155,18
	1237	ŏ	LYS C	154	21.927	14.291	19.599	1.00	155.19
	1238	Ň	VAL C	155	22,410	15.798	17.993	1.00	207.77
	1239	CA	VAL C	155	21.031	16.198	17.727	1.00	207.77
55	1240	CB	VAL C	155	20.918	17.729	17.614	1.00	240.62
	1241	CG1	VAL ٽِ	155	19.500	18.129	17.274	1.00	240.62
	1242	CG2	VAL C	155	21.336	18.369	18.918	1.00	240.62
	1243	C	VAL C	155	20.663	15.572	16.392 15.410	1.00 1.00	207.77 207.77
60	1244	0	VAL C TRP C	155	21.387 19.536	15.758 14.860	16.343	1.00	218.56
oo	1245 1246	N CA	TRP C	156 156	19.108	14.172	15.113	1.00	218.56
	1247	CB	TRP C	156	19.013	15.124	13.897	1.00	249.69
	1248	CG	TRP C	156	17.915	16.165	13.921	1.00	249.69
	1249	CD2	TRP C	156	16.500	15.936	13.835	1.00	249.69
65	1250	CE2	TRP C	156	15.869	17.203	13.878	1.00	249.69
	1251	CE3	TRP C	156	15.705	14.788	13.725	1.00	249.69
	1252	CD1	TRP C	156	18.077	17.523	14.010	1.00 1.00	249.69 249.69
	1253	NE1	TRP C	156 156	16.854 14.481	18.152 17.354	13.983 13.816	1.00	249.69
70	1254 1255	CZ2 CZ3	TRP C	156 156	14.324	14.939	13.660	1.00	249.69
70	1233	مص	iiie o			, ,,,,,,,			

	1256	CH2	TRP C	156	13.728	16.214	13.709	1.00	249.69
	1257	C C	TRP C	156	20.213	13.163	14.835	1.00	218.56
	1258	ŏ	TRP C	156	20.243	12.080	15.416	1.00	218.56
	1259	Ň	GLN C	157	21.130	13.548	13.949	1.00	165.87
5	1260	CA	GLN C	157	22.264	12.707	13.578	1.00	165.87
•	1261	СВ	GLN C	157	21.918	11.902	12.321	1.00	216.87
	1262	CG	GLN C	157	20.967	10.737	12.583	1.00	216.87
	1263	CD	GLN C	157	21.564	9.669	13.496 13.154	1.00 1.00	216.87 216.87
	1264	OE1	GLN C	157	22.561	9.032 9.468	14.661	1.00	216.87
10	1265	NE2	GLN C	157	20.951	9.400 13.461	13.378	1.00	165.87
	1266	Ç	GLN C	157	23.592 24.495	12.979	12.705	1.00	165.87
	1267	0	GLN C LEU C	157 158	23.706	14.648	13.960	1.00	219.11
	1268	N CA	LEU C	158	24.940	15.419	13.858	1.00	219.11
15	1269	CA CB	LEU C	158	24.767	16.628	12.929	1.00	248.45
13	1270 1271	CG	LEU C	158	24.766	16.392	11.415	1.00	248.45
	1272	CD1	LEU C	158	25.460	17.580	10.748	1.00	248.45
	1273	CD2	LEU C	158	25.498	15.110	11.054	1.00	248.45
	1274	C	LEU C	158	25.415	15.892	15.230	1.00	219.11
20	1275	0	LEU C	158	24.619	16.116	16.136	1.00	219.11
	1276	N	ASP C	159	26.724	16.040	15.374	1.00 1.00	202.98 202.98
	1277	CA	ASP C	159	27.314	16.485	16.629 16.757	1.00	249.69
	1278	CB	ASP C	159	28.746	15.957 14.458	16.563	1.00	249.69
0.5	1279	CG	ASP C	159	28.834 28.215	13.718	17.356	1.00	249.69
25	1280	OD1	ASP C ASP C	159 159	29.522	14.017	15.616	1.00	249.69
	1281	OD2	ASP C	159	27.341	18.007	16.704	1.00	202.98
	1282	C O	ASP C	159	27.474	18.690	15.682	1.00	202.98
	1283 1284	Ň	TYR C	160	27.209	18.541	17.915	1.00	193.11
30	1285	CA	TYR C	160	27.246	19.988	18.104	1.00	193.11
50	1286	CB	TYR C	160	25.852	20.584	18.043	1.00	187.38
	1287	CG	TYR C	160	25.114	20.253	16.778	1.00	187.38
	1288	CD1	TYR C	160	24.305	19.113	16.702 15.553	1.00 1.00	187.38 187.38
	1289	CE1	TYR C	160	23.579	18.813	15.665	1.00	187.38
35	1290	CD2	TYR C	160	25.195	21.087 20.796	14.504	1.00	187.38
	1291	CE2	TYR C	160	24.479 23.666	19.657	14.458	1.00	187.38
	1292	CZ	TYR C TYR C	160 160	22.920	19.374	13.337	1.00	187.38
	1293	ОН	TYR C	160	27.895	20.388	19.413	1.00	193.11
40	1294 1295	CO	TYR C	160	27.769	19.705	20.429	1.00	193.11
40	1295	Ň	GLU C	161	28.585	21.519	19.360	1.00	171.02
	1297	CA	GLU C	161	29.296	22.064	20.494	1.00	171.02
	1298	CB	GLU C	161	30.740	22.358	20.052	1.00	238.76
	1299	CG	GLU C	161	31.660	22.975	21.085	1.00	238.76 238.76
45	1300	CD	GLU C	161	33.121	22.878	20.671 21.196	1.00 1.00	238.76
	1301	OE1	GLU C	161	33.948	23.655	19.827	1.00	238.76
	1302	OE2	GLU C	161	33.445	22.015 23.321	20.952	1.00	171.02
	1303	C	GLU C	161 161	28.560 28.044	24.068	20.135	1.00	171.02
50	1304	0	GLU C SER C	162	28.500	23.533	22.263	1.00	160.21
30	1305 1306	N CA	SER C	162	27.820	24.693	22.840	1.00	160.21
	1307	CB	SER C	162	27.182	24.308	24.174	1.00	143.02
	1308	OG	SER C	162	28.169	23.903	25.109	1.00	143.02
	1309	Č	SER C	162	28.767	25.856	23.078	1.00	160.21
55	1310	Ō	SER C	162	29.978	25.678	23.147	1.00	160.21
•-	1311	N	GLU C	163	28.211	27.053	23.200	1.00	142.78 142.78
	1312	CA	GLU C	163	29.043	28.207	23.471	1.00 1.00	247.65
٠	1313	CB	GLU C	163	28.195	29.492	23.498 22.130	1.00	247.65
	1314	CG	GLU C	163		30.009 30,651	21.331	1.00	247.65
60	1315	CD	GLU C	163 163		31.604	21.841	1.00	247.65
	1316	OE1	GLU C	163		30.207	20.189	1.00	247.65
	1317 1318	OE2 C	GLU C	163		27.931	24.857	1.00	142.78
	1319	ŏ	GLU C	163		27.254	25.666	1.00	142.78
65	1320	N	PRO C	164		28.429	25.144	1.00	104.76
03	1321	CD	PRO C	164		29.158	24.241	1.00	198.66
	1322	CA	PRO C	164		28.209	26.442	1.00	104.76
	1323	СВ	PRO C	164		28.445	26.144	1.00	198.66 198.66
	1324	ÇG	PRO C	164		29.581	25.180 27.501	1.00 1.00	104.76
70	1325	С	PRO C	164	30.943	29.170	27.501	1.00	104.10

	1326 1327	O N		165	30.623 30.872 30.352	30.318 28.719 29.562	27.189 28.751 29.820	1.00 1.00 1.00	104.76 150.81 150.81
	1328	CA: CB	LEU C	165	28.962	29.067	30.202 31.329	1.00 1.00	114.56 114.56
5	1329 1330	ca	LEU C		28.295	29.843 31.336	31.179	1.00	114.56
5	1331	CD1	LEU C		28.627 26.778	29.5°C	31.296	1.00	114.56
	1332	CD2	LEU C	165 165	31.213	29.644	31.065	1.00	150.81
	1333	CO	LEU C	165	31.648	28.620	31.589	1.00 1.00	150.81 123.03
10	1334 1335	N	ASN C	166	31.445	30.864	31.538 32.744	1.00	123.03
10	1336	CA	ASN C	166	32.247	31.058 32.409	32.716	1.00	146.40
	1337	CB	ASN C	166 166	32.969 34.388	32.314	32.177	1.00	146.40
	1338	CG	ASN C ASN C	166	35.031	31.273	32.254	1.00	146.40 146.40
15	1339	OD1 ND2	ASN C	166	34.888	33.429	31.660 34.019	1.00 1.00	123.03
15	1340 1341	C	ASN C	166	31.402	30.985 31.409	34.022	1.00	123.03
	1342	Ö	ASN C	166	30.257 31.976	30.458	35.103	1.00	149.03
	1343	N.	ILE C	167 167	31.266	30.320	36.374	1.00	149.03
00	1344	CA CB	ILE C	167	30.670	28.946	36.551	1.00 1.00	98.22 98.22
20	1345 1346	CG2	ILE C	167	30.085	28.799	37.947 35.473	1.00	98.22
	1347	CG1	ILE C	167	29.610	28.707 27.336	35.526	1.00	98.22
	1348	CD1	ILE C	-167 167	29.025 32.178	30.592	37.548	1.00	.149.03
	1349	C	ILE C	167	33.233	29.983	37.667	1.00	149.03 107.43
25	1350	0 N	THR C	168	31.755	31.471	38.440 39.591	1.00 1.00	107.43
	1351 1352	CA	THR C	168	32.586	31.792 33.225	39.487	1.00	120.91
	1353	CB	THR C	168	33.120 33.823	33.372	38.246	1.00	120.91
	1354	OG1	THR C	168 168	34.054	33.526	40.533	1.00	120.91
30	1355	CG2 C	THR C	168	31.955	31.603	40.965 41.312	1.00 1.00	107.43 107.43
	1356 1357	ŏ	THR C	168	30.943	32.192 30.761	41.750	1.00	107.46
	1358	N	VAL C	169	32.594 32.152	30.470	43.092	1.00	107.46
	1359	CA	VAL C VAL C	169 169	32,206	28.935	43.374	1.00	105.06 105.06
35	1360	CB CG1	VAL C	169	32.281	28.657	44.853	1.00 1.00	105.06
	1361 1362	CG2	VAL C	169	30.966	28.269	42.794 44.025	1.00	107.46
	1363	C	VAL C	169	33.083	31,217 30,874	44.135	1.00	107.46
	1364	0	VAL C	169 170	34.266 32.548	32.248	44.677	1.00	143.55
40	1365	N	ILE C	170	33.320	33.068	45.614	1.00	143.55 150.86
	1366 1367	CA CB	ILE C	170	32.910	34.549	45.488 44.028	1.00 1.00	150.86
	1368	CG2	ILE C	170	32.957	34.967 34.741	46.000	1,00	150.86
	1369	CG1	ILE C	170 170		36,188	45.961	1.00	150.86
45		CD1	ILE C	170		32.586	47.056	1.00 1.00	143.55 143.55
	1371	CO	ILE C	170	32.173	31.824	47.309 47.994	1.00	170.19
	1372 1373	Ň	LYS C	171		33.028 32.588	49.379	1.00	170.19
	1374	CA	LYS C	171		31.812	49.790	1.00	247.79
50		CB	LYS C	171 171		32.611	49.598	1.00	247.79 247.79
	1376	CD CD	LYS C	17		31.712	49.375 50.537	1.00 1.00	247.79
	1377 1378	CE	LYS C	17		30.756 29.921	50.335	1.00	247.79
	1379	NZ	LYS C	17		33.715	50.378	1.00	170.19
5:	5 1380	C	LYS C	17 [.] 17		33.498	51.596	1.00	170.15 249.69
	1381	0 C1	NAG C	22	*	30.265	25.361 25.132	1.00 1.00	249.69
	1382 1383	C2	NAG C	22	1 5.275	28.765	24.798		249.69
	1384	N2	NAG C	22		28.481 27.267	25.015		249.69
6	0 1385	C7	NAG C	22 22		26.331	25.485		249.69 249.69
	1386	O7 C8	NAG C NAG C			27.050	24.648		249.69
	1387 1388	čŝ	NAG C	22	1 4.349	28.288	24.010 23.92		249.69
	1389	Õŝ	NAG C	22		26.868 28.741	24.22		249.69
6	5 1390	C4	NAG C		21 2.899 21 2.183	28.474	23.00	2 1.00	249.69
	1391	O4 C5	NAG C		21 2.851	30.255	24.55		249.69 249.69
	1392	C5 O5	NAG C		21 3.741	30.568	25.65 24.97		249.69
	1393 1394	C6	NAG C	, 2	21 1.472	30.743 30.009	26.08		249.69
•	70 1395	06	A NAG	; 2	21 0.977	30.003			

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	1396 1397	C1 C2	NAG C NAG C	222 222	0.788	28.434	23.006	1.00	249.69
	1398	N2.	NAG C	222	0.312 0.806	27.230 25.988	22.166 22.749	1.00	249.69
_	1399	C7	NAG C	222	-0.041	25.044	23.166	1.00 1.00	249.69 249.69
5	1400	07	NAG C	222	-1.270	25,153	23.088	1.00	249.69
	1401	C8	NAG C	222	0.570	23.783	23.761	1.00	249.69
	1402 1403	C3 O3	NAG C NAG C	222 222	0.819 0.285	27.382	20.711	1.00	249.69
	1404	C4	NAG C	222	0.422	26.347 28.755	19.894 20.130	1.00	249.69
10	1405	04	NAG C	222	1.038	28.935	18.860	1.00 1.00	249.69 249.69
	1406	Ç5	NAG C	222	0.860	29.881	21.083	1.00	249.69
	1407 1408	O5 C6	NAG C	222	0.308	29.658	22.408	1.00	249.69
	1408	O6	NAG C NAG C	222 222	0.423 1.512	31.266	20.635	1.00	249.69
15	1410	C1	NAG C	242	18.968	32.185 46.404	20.656 25.932	1.00 1.00	249.69
	1411	C2	NAG C	242	18.118	46.230	24.662	1.00	249.69 249.69
	1412	N2	NAG C	242	16.700	46.211	24.968	1.00	249.69
	1413 1414	C7 O7	NAG C NAG C	242	15.905	47.139	24.446	1.00	249.69
20	1415	∵8	NAG C	242 242	16.318 14.433	48.033 47.071	23.707	1.00	249.69
	1416	C3	NAG C	242	18.532	44.931	24.794 23.964	1.00 1.00	249.69 249.69
	1417	Q3	NAG C	242	17.775	44.760	22.773	1.00	249.69
	1418 1419	C4	NAG C	242	20.036	44.983	23.636	1.00	249.69
25	1420	O4 C5	NAG C NAG C	242 242	20.457	43.699	23.125	1.00	249.69
	1421	O5	NAG C	242	20.872 20.352	45.340 46.526	24.894 25.559	1.00	249.69
	1422	C6	NAG C	242	22.318	45.643	24.539	1.00 1.00	249.69 249.69
	1423	06	NAG C	242	23.194	44.624	24.998	1.00	249.69
30	1424 1425	C1 C2	NAG C	243	21.000	43.678	21.849	1.00	249.69
50	1426	N2	NAG C NAG C	243 243	21.827 22.908	42.403 42.331	21.660	1.00	249.69
	1427	C7	NAG C	243	23.110	41.201	22.621 23.298	1.00 1.00	249.69
	1428	07	NAG C	243	22.404	40.193	23.157	1.00	249.69 249.69
35	1429 1430	C8	NAG C	243	24.264	41.186	24.287	1.00	249.69
55	1431	C3 O3	NAG C NAG C	243 243	22.382 23.150	42.377	20.246	1.00	249.69
	1432	C4	NAG C	243	21.223	41.195 42.406	20.045 19.276	1.00 1.00	249.69
	1433	04	NAG C	243	21.794	42.333	17.983	1.00	249.69 249.69
40	1434	C5	NAG C	243	20.366	43.682	19.518	1.00	249.69
+0	1435 1436	O5 C6	NAG C NAG C	243 243	19.915	43.690	20.906	1.00	249.69
	1437	06	NAG C	243	19.112 18.229	43.738 42.666	18.662 18.966	1.00	249.69
	1438	C1	MAN C	244	21.150	41.717	16.941	1.00 1.00	249.69 247.75
45	1439	C2	MAN C	244	21.485	42.608	15.841	1.00	247.75
45	1440 1441	O2 C3	MAN C	244	22.880	42.966	15.943	1.00	247.75
	1442	03	MAN C MAN C	244 244	21.041 21.229	42.012 42.927	14.541	1.00	247.75
	1443	C4	MAN C	244	21.699	40.671	13.482 14.305	1.00 1.00	247.75
50	1444	04	MAN C	244	21.301	40.157	13.050	1.00	247.75 247.75
50	1445 1446	C5	MAN C	244	21.269	39.743	15.442	1.00	247.75
	1447	O5 C6	MAN C MAN C	244 244	21.734 21.705	40.330	16.721	1.00	247.75
	1448	06	MAN C	244	23.038	38.271 38.030	15.255 15.676	1.00 1.00	247.75
	1449	C1	NAG C	250	0.024	39.200	37.140	1.00	247.75 249.69
55	1450	C2	NAG C	250	-0.633	37.995	37.P 14	1.00	249.69
	1451 1452	N2 C7	NAG C	250	-0.363	38.033	39.271	1.00	249.69
	1453	07 07	NAG C NAG C	250 250	-1.342 -2.500	38.313 38.550	40.126	1.00	249.69
	1454	C8	NAG C	250	-0.985	38.336	39.764 41.607	1.00 1.00	249.69
60	1455	C3	NAG C	250	-0.084	36.691	37.242	1.00	249.69 249.69
	1456 1457	O3	NAG C	250	-0.751	35.573	37.814	1.00	249.69
	1457	C4 O4	NAG C NAG C	250 250	-0.273	36.691	35.716	1.00	249.69
	1459	C5	NAG C	250 250	0.355 0.338	35.542 37.973	35.160 35.105	1.00	249.69
65	1460	O 5	NAG C	250	-0.235	39.149	35.731	1.00 1.00	249.69 249.69
	1461	C6	NAG C	250	0.100	38.106	33.606	1.00	249.69
	1462 1463	O6 C1	NAG C	250	0.341	39.435	33.163	1.00	249.69
	1464	C2	NAG C NAG C	274 274	17.463 18.624	53.378 52.801	50.102	1.00	249.69
70	1465	N2	NAG C	274	18.123	51.805	50.945 51.883	1.00 1.00	249.69
							5500	1.00	249.69

			NAC C	27,4	18.919	50.834	52.330	1.00	249.69
	1466	C7	NAG C NAG C		20.099	50.723	51.992	1.00	249.69
	1467	07 C8.	DAM C		18.316	49.836	53.303	1.00	249.69
	1468 1469	C3	NAG C	274	19.337	53.945	51.704	1.00 1.00	249.69 249.69
5	1470	03	NAG C		20.487	53.442	52.377 50.730	1.00	249.69
3	1471	C4	NAG C	274	19.755	55.062 56.164	51,457	1.00	249.69
	1472	04	NAG C	274	20.286	55.520	49.899	1.00	249.69
	1473	C5	NAG C	274 274	18.548 17.957	54.391	49.203	1.00	249.69
	1474	O5	NAG C NAG C	274	18.929	56.550	48.849	1.00	249.69
10	1475	C6 O6	NAG C	274	17.844	56.817	47.970	1.00	249.69
	1476 1477	C1	NAG C	335	16.958	19.435	32.669	1.00	249.69 249.69
	1477	C2	NAG C	335	15.937	19.674	33.820 35.073	1.00 1.00	249.69
	1479	N2	NAG C	335	16.535	19.244	36.042	1.00	249.69
15	1480	C7	NAG C	335	16.783	20.124 21.327	35.947	1.00	249.69
	1481	07	NAG C	335	16.517 17.416	19.588	37.314	1.00	249.69
	1482	C8	NAG C NAG C	335 335	14.586	18.951	33.638	1.00	249.69
	1483	C3	NAG C	335	13.605	19.572	34.457	1.00	249.69
20	1484	O3 C4	NAG C	335	14,117	18.995	32.190	1.00	249.69
20	1485 1486	O4	NAG C	335	12.912	18.250	32.042	1.00	249.69 249.69
	1487	C5	NAG C	335	15.219	18.405	31.318	1.00 1.00	249.69
	1488	O 5	NAG C	335	16.370	19.273	31.353 29.862	1.00	249.69
	1489	C6	NAG C	335	14.799	18.275	29.398	1.00	249.69
25	1490	O6	NAG C	335	14.956	16.942 21.246	52.250	1.00	249.46
	1491	C1	NAG C	340 340	29.647 30.433	22.313	53.032	1.00	249.46
	1492	C2	NAG C NAG C	340	30.974	23.304	52.117	1.00	249.46
	1493	N2	NAG C	340	30.836	24.605	52.373	1.00	249.46
20	1494	C7 O7	NAG C	340	30.269	25.044	53.381	1.00	249.46
30	1495 1496	C8	NAG C	340	31.425	25.569	51.356	1.00	249.46 249.46
	1490	C3	NAG C	340	31.568	21.625	53.818 54.628	1.00 1.00	249.46
	1498	03	NAG C	340	32.255	22.575	54.702	1.00	249.46
	1499	C4	NAG C	340	30.996	20.503 19.789	55.308	1.00	249.46
35	1500	O4	NAG C	340	32.063 30.136	19.545	53.853	1.00	249.46
	1501	C5	NAG C	340 340	29.101	20.280	53.154	1.00	249.46
	1502	O5	NAG C	340	29.442	18.463	54.660	1.00	249.46
	1503	C6 O6	NAG C	340	28.518	17.737	53.851	1.00	249.46
40	1504 1505	C1	NAG C	366	36.171	33.414	30.999	1.00	209.37 209.37
40	1506	G2	NAG C	366	38.136	34.345	29.797 28.886	1.00 1.00	209.37
	1507	N2	NAG C	366	35.092	33.912	28.999	1.00	209.37
	1508	C7	NAG C	366	33.862	34.405 35,244	29.848	1.00	209.37
	1509	07	NAG C	366	33.555 32.813	33.903	28.017	1.00	209.37
45	1510	C8	NAG C NAG C	366 366	37.487	34.322	29.088	1.00	209.37
	1511	C3 C3	NAG C	366	37.518	35.319	28.073	1.00	209.37
	1512	O3 C4	NAG C	366		34.557	30.067	1.00	209.37
	1513 1514	64	NAG C	366	39.884	34.256	29.386	1.00 1.00	209.37 209.37
50	1515	C5	NAG C	366		33.652	31.302 31.891	1.00	209.37
50	1516	O 5	NAG C	366		33.813	32.390	1.00	209.37
	1517	C6	NAG C	366		33,935 32,957	33.413	1.00	209.37
	1518	Q 6	NAG C	366		35.232	29.397	1.00	249.69
	1519	C1	NAG C NAG C	367 367		34.596	29.111	1.00	249.69
55		C2	NAG C	367		33.546	30.070	1.00	249.69
	1521	N2 C7	NAG C	367		32.277	29.668	1.00	249.69
	1522 1523	07	NAG C	367		31.931	28.498	1.00	249.69 249.69
	1523	C8	NAG C	367		31.227	30.725	1.00 1.00	249.69
60	1525	C3	NAG C			35.695	29.166 28.892	1.00	249.69
-	1526	03	NAG C			35.149 36.779	28.132		249.69
	1527	C4	NAG C			37.854	28.245		249.69
	1528	04	NAG C			37.296	28.348		249.69
_	1529	C5	NAG C			36.196	28.373	1.00	249.69
6:	5 1530	O5	NAG C NAG C			38.236	27.251		249.69
	1531	C6 O6	NAG C			37.661	26.474		249.69
	1532 1533	CB	LYS A	_	3.684	19.933	14.932		249.69 249.69
	1534	ca	LYS A	4	2.729	21.022	14.456 15.610		249.69
7	0 1535	CD		4	2.217	21.880	15.61	, 1.00	2,2,44
•					•				

	1536	CE	LYS A	4.	1.292	22.987	15.108	1.00	249.69
	1537	NZ	LYS A	4	0.762	23.841	16.212	1.00	249.69
	1538	C ·	LYS A	4	5.030	20.019	12.832	1.00	249.22
	1539	o ·	LYS A	4	5.450	21.116	13.205	1.00	249.22
5	1540	N	LYS A	4	5.205	18.061	14.356	1.00	249.22
	1541	CA	LYS A	4	4.291	19.100	13.797	1.00	249.22
	1542	N	PRO A	5	5.213	19.581	11.582	1.00	249.41
	1543	CD	PRO A	5	4.979	18.215	11.068	1.00	133.18
	1544	CA	PRO A	5	5.912	20.398	10.589	1.00	249.41
10	1545	СВ	PRO A	5	6.459	19.360	9.606	1.00	133.18
	1546	CG	PRO A	5	5.376	18.335	9.599	1.00	133.18
	1547	С	PRO A	5	4.969	21.407	9.927	1.00	249.41
	1548	0	PRO A	5	3.754	21.219	9.927	1.00	249.41
_	1549	N	LYS A	6	5.529	22.477	9.377	1.00	196.60
15	1550	CA	LYS A	6	4.724	23.489	8.709	1.00	196.60
	1551	CB	LYS A	6	4.429	24.652	9.660	1.00	249.69
	1552	CG	LYS A	6	3.524	25.719	9.050	1.00	249.69
	1553	CD	LYS A	6	3.113	26.783	10.067	1.00	249.69
	1554	CE	LYS A	6	2.180	27.812	9.436	1.00	249.69
20	1555	NZ	LYS A	6	1.664	28.800	10.424	1.00	249.69
	1556	C	LYS A	6	5.433	24.000	7.458 7.530	1.00	196.60
	1557	0	LYS A	6	6.478	24.664	7.539	1.00	196.60 192.34
	1558	N.	VAL A	7	4.850	23.695	6.304	1.00	
05	1559	CA	VAL A	7	5.416	24.094	5.029 3.870	1.00 1.00	192.34 160.27
25	1560	CB	VAL A	7	4.656	23.429	2.587	1.00	160.27
	1561	CG1	VAL A	7	5.470	23.549 21.983	4.195	1.00	160.27
	1562	CG2	VAL A	7	4.363 5.403	25.607	4.807	1.00	192.34
	1563	C	VAL A	7 7	4.350	26.253	4.868	1.00	192.34
20	1564	O.	VAL A SER A	8	6.582	26.165	4.544	1.00	184.23
30	1565	N CA	SER A	8	6.726	27.594	4.284	1.00	184.23
	1566	CA	SER A	8	7.897	28.148	5.099	1.00	230.08
	1567	CB OG	SER A	8	9.063	27.354	4.945	1.00	230.08
	1568	C	SER A	8	6.978	27.814	2.789	1.00	184.23
35	1569	ŏ	SER A	8	7.389	26.889	2.087	1.00	184.23
33	1570 1571	N	LEU A	9	6.726	29.025	2.297	1.00	167.11
	1572	CA	LEU A	9	6.948	29.312	0.880	1.00	167.11
	1573	CB	LEU A	9	5.626	29.535	0.147	1.00	178.21
	1574	ÇG.	LEU A	9	4.541	28.451	0.105	1.00	178.21
40	1575	CD1	LEU A	9	3.549	28.821	-0.980	1.00	178.21
40	1576	CD2	LEU A	9	5.128	27.083	-0.188	1.00	178.21
	1577	C	LEU A	9	7.817	30.533	0.666	1.00	167.11
	1578	ŏ	LEU A	9	7.946	31.373	1.552	1.00	167.11
	1579	Ň	ASN A	10	8.405	30.629	-0.522	1.00	147.32
45	1580	CA	ASN A	10	9.260	31.769	-0.855	1.00	147.32
	1581	CB	ASN A	10	10.634	31.610	-0.219	1.00	249.69
	1582	CG	ASN A	10	11.421	32.902	-0.234	1.00	249.69
	1583	OD1	ASN A	10	11.028	33.886	0.395	1.00	249.69
	1584	ND2	ASN A	10	12.534	32.911	-0.959	1.00	249.69
50	1585	С	ASN A	10	9.396	31.902	-2.374	1.00	147.32
	1586	0	ASN A	10	10.037	31.073	-3.022	1.00	147.32
	1587	N	PRO A	11	8.851	32.979	-2.953	1.00	237.62
	1588	CD	PRO A	11	8.944	33.177	-4.413	1.00	161.80
	1589	CA	PRO A	11	8.057	34.058	-2.348	1.00	237.62
55	1590	СВ	PRO A	11	7.554	34.834	-3.552	1.00	161.80
	1591	CG	PRO A	11	8.646	34.638	-4.548	1.00	161.80
	1592	Ç	PRO A	11	6.921	33.599	-1.438	1.00	237.62
	1593	0	PRO A	11	6.554	32.428	-1.435	1.00	237.62
	1594	N	PRO A	12	6.338	34.529	-0.662	1.00	147.54
60	1595	CD	PRO A	12	6.781	35.905	-0.441	1.00	140.19
	1596	CA	PRO A	12	5.229	34.189	0.236	1.00	147.54
	1597	CB	PRO A	12	5.107	35.433	1.112	1.00	140.19 140.19
	1598	ÇG	PRO A	12	6.465	38.081	1.016	1.00 1.00	140.19
25	1599	C	PRO A	12	3.967	33.943	-0.572 -0.148	1.00	147.54
65	1600	0	PRO A	12	3.063	33.202 34.576	-0.148 -1.744	1.00	165.94
	1601	N	TRP A	13	3.929	34.576 34.492	-1.7 44 -2.698	1.00	165.94
	1602	CA	TRP A	13	2.824 3.247	34.492 35.209	-2.096 -3.968	1.00	139.27
	1603	CB CG	TRP A	13 13	3.825	36.552	-3.699	1.00	139.27
70	1604 1605	CD2	TRP A	13	3.455	37.438	-2.648	1.00	139.27
70	1003	CUZ	THE A	10	0.400	37.730	~2.040		109.27

	1606 1607	CE2 CE3		13 13	4.233 2.546	38.603 37.363	-2.790 -1.594 -4.428	1.00 1.00 1.00	139.27 139.27 139.27
	1608	CD1	TRP A	13	4.784	37.201 38.438	-3.891	1.00	139.27
	1609	NE1.	TRP A	13	5.035 4.122	39.682	-1.917	1.00	139.27
5	1610	CZ2	TRP A	13 13	2.433	38.434	-0.731	1.00	139.27
	1611	CZ3	TRP A	13	3.218	39.577	-0.892	1.00	139.27
	1612	CH2	TRP A	13	2.428	33.061	-3.048	1.00 1.00	165.94 165.94
	1613	C	TRP A	13	3.219	32.342	-3.663 -2.689	1.00	109.00
10	1614 1615	N	ASN A	14	1.213	32.652	-2.990	1.00	109.00
10	1616	CA	ASN A	14	0.782	31.293 30.660	-1.746	1.00	167.27
	1617	CB	ASN A	14	0.167 -1.091	31.352	-1.312	1.00	167.27
	1618	CG	ASN A	14 14	-1.088	32,556	-1.050	1.00	167.27
	1619	OD1	ASN A ASN A	14	-2.188	30.596	-1.234	1.00	167.27 109.00
15	1620	ND2 C	ASN A	14	-0.200	31.224	-4.164 -4.295	1.00 1.00	109.00
	1621 1622	ŏ	ASN A	14	-0.981	30.275	-5.006	1.00	160.32
	1623	Ň	ARG A	15	-0.153	32.255 32.384	-6.220	1.00	160.32
	1624	CA	ARG A	15	-0.977 -2.094	33.426	-6.042	1.00	119.95
20	1625	CB	ARG A ARG A	15 15	-2.974	33.286	-4.790	1.00	119.95
	1626	CG	ARG A	15	-4.127	34.296	-4.834	1.00	119.95 119.95
	1627	CD NE	ARG A	15	-5.205	33.881	-5.737 6.500	1.00 1.00	119.95
	1628 1629	CZ	ARG A	15	-5.920	34.709	-6.500 -6.492	1.00	119.95
25	1630	NH1	ARG A	15	-5.674	36.015 34.239	-7.267	1.00	119.95
	1631	NH2	ARG A	15	-6.894 0.012	32.914	-7.260	1.00	160.32
	1632	Ç	ARG A	15 15	0.338	34.098	-7.259	1.00	160.32
	1633	0	ARG A ILE A	16	0.490	32.054	-8.148	1.00	135.68 135.68
20	1634	N CA	ILE A	16	1.479	32.491	-9,124 -8.904	1.00 1.00	134.22
30	1635 1636	CB	ILE A	16	2.803	31,783 32,401	-7.704	1.00	134.22
	1637	CG2	ILE A	16	3.532 2.534	30.272	-8.762	1.00	134.22
	1638	CG1	ILE A	16 16	3.763	29.404	-8.762	1.00	134.22
	1639	CD1	ILE A ILE A	16	1.141	32.283	-10.581	1.00	135.68 135.68
35	1640	CO	ILE A	16	0.358	31.408	-10.938 -11.425	1.00 1.00	145.71
	1641 1642	Ň	PHE A	17	1.774	33.090	-12.870	1.00	145.71
	1643	CA	PHE A	17	1.589	33.015 34.246	-13.547	1.00	146.10
	1644	CB	PHE A	17	2.211 1.276	35.401	-13.687	1.00	146.10
40	1645	CG	PHE A	17 17	1.752	36.702	-13.601	1.00	146.10
	1646	CD1	PHE A PHE A	17	-0.067	35.195	-13.957	1.00	146.10 146.10
	1647	CD2 CE1	PHE A	17	0.901	37.798	-13.781 -14.142	1.00 1.00	146.10
	1648 1649	CE2	PHE A	17	-0.927	36.273 37.586	-14.054	1.00	146.10
45	1650	CZ	PHE A	17	-0.437	31.7 44	-13.417	1.00	145.71
-10	1651	С	PHE A	17	2.240 2.882	30.991	-12.692	1.00	145.71
	1652	0	PHE A LYS A	17 18	2.074	31.534	-14.713	1.00	190.00 190.00
	1653	N GA	LYS A	18	2.625	30.380	-15.402	1.00 1.00	249,19
50	1654) 1655	CB	LYS A	18	1.798	30.115	-16.669 -17.483	1.00	249.19
50	1656	ČĠ	I.YS A	18	2.212	28.904 28.655	-18.601	1.00	249.19
	1657	CD	LYS A	18	1.206	27.498	-19,493	1.00	249.19
	1658	CE	LYS A	18 18	1.619 2.837	27.814	-20.292	1.00	249.19 190.00
_	1659	NZ	LYS A LYS A	18	4,101	30.602	-15.765	1.00 1.00	190.00
5	5 1660 1661	CO	LYS A	18	4.472	31.613	-16.368 -15.390		217.86
	1662	Ň	GLY A	19	4.945	29.648 29.759	-15.698		217.86
	1663	CA	GLY A	19	6.356	30.324	-14.582		217.86
	1664	Ç	GLY A		7.219 8.449	30.261	-14.675		217.86
6	0 1665	0	GLY A GLU A			30.874	-13.537	1.00	170.23 170.23
	1666	N CA	GLU A			31.452	-12.399		186.84
	1667 1668	CB	GLU A		6.435	32.409	-11.611 -12.440		186.84
	1669	čG	GLU A	20		33.418 34.410	-11.57		188.84
6	5 1670	CD	GLU A			33.972	-10.68	1.00	186.84
	1671	OE1	GLU A			35.633	-11.79		186.84
	1672	OE2	GLU A			30.341	-11.45		170.23 170.23
	1673	CO	GLU /		7.274	29.232	-11.46		187.01
	1674 70 1675	N	ASN			30.634	-10.63	0 1.00	
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•							-9.707	1.00	187.01
4.6	576	CA	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	21	9.372	29.622 29.456	-9.859	1.00	249.69
	370 377	CB	,	21 21	10.888 11.371	29.621	-11.291	1.00	249.69 249.69
10	678	CG	ASN A ASN A	21	10.828	29.039	-12.233 -11.435	1.00 1.00	249.69
- 11	679	OD1 ND2	ASN A	21	12.423	30.420	-8.230	1.00	187.01
	680 681	C	ASN A	21	9.087	29.907 51.054	-7.786	1.00	187.01
	681 682	ŏ	ASN A	21	9.136 8.816	28.842	-7.477	1.00	223.09
i	683	N	VAL A	22 22	8.516	28.936	-6.050	1.00 1.00	223.09 159.07
1	1684	CA	VAL A	22	6.995	28.809	-5.785 -6.039	1.00	159.07
	1685	CB CG1	VAL A	22	6.530	27.388 29.212	-4.363	1.00	159.07
	1686 1687	CG2	VAL A	22	6.680	29.212 27.825	-5 280	1.00	223.09
	1688	c c	VAL A	22	9.228 9.418	26.731	-5.801	1.00	223.09 162.43
	1689	0	VAL A THR A	22 23	9.600	28.102	-4 033 2 407	1.00 1.00	162.43
	1690	N	THR A	23	10.307	27.125	-3.197 -2.758	1.00	218.62
	1691	CB CA	THR A	23	11.677	27.680 28.165	-3.905	1.00	218.62
	1692 1693	OG1	THR A	23	12.384	26.594	-2.071	1.00	218.62
	1694	CG2	THR A	23 23	12.498 9.549	26.715	-1.924	1.00	162.43 162.43
20	1695	C	THR A THR A	23	9.185	27.571	-1.114 -1.736	1.00 1.00	159.52
	1696	0 N	LEU A	24	9.337	25.410	-0.549	1.00	159.52
	1697	CA	LEU A	24	8.635	24.916 23.860	-0.923	1.00	128.43
	1698 1699	CB	LEU A	24	7.593 6.845	23.919	-2.252	1.00	128.43 128.43
25	1700	CG	LEU A	24 24	5.664	22.963	-2.175	1.00 1.00	128.43
	1701	CD1	LEU A LEU A	24	6.352	25.322	-2.557 0.464	1.00	150.52
	1702	CD2 C	LEU A	24	9.600	24.299 23.201	0.247	1.00	159.52
	1703 1704	ŏ	LEU A	24	10.111	24.999	1.574	1.00	201.17
30	1705	N	THR A	25	9.827 10.722	24.533	2.637	1.00	201.17 221.92
50	1706	CA	A SHIT	25 25	11.524	25.712	3,227	1.00 1.00	221.92
	1707	CB OG1	THR A	25	12.249	26.363	2.178 4.293	1.00	221.92
	1708	CG2	THR A	25	12.501	25. 22 5 23.875	3.767	1.00	201.17
35	1709 1710	Č	THR A	25	9.919 8.912	24.429	4.215	1.00	201.17 178.89
33	1711	0	THR A	25 26	10.363	22.707	4.232	1.00 1.00	178.89
	1712	N	CYS A	26	9.668	21.995	5.311 6.672		178.89
	1713	CA C	CYS A	26	10.061	22.556 22.904	6.885		178.89
40	1714 1715	ŏ	CYS A	26	11.220	20.504	5.257	1.00	171.78
40	1716	СВ	CYS A	26		19.467	6.366		171.78 234.74
	1717	SG	CYS A ASN A	26 27		22.623	7.589		234.74
	1718	N	ASN A	27	9.307	23.180	8.929 9.987		249.69
AE	1719	CA CB	ASN A	27		22.337 23.020	11.35	1.00	249.69
45	1720 1721	čĞ	ASN A	27		24,193	11.46	3 1.00	249.69 2 i 9.69
	1722	OD1	ASN A			22.284	12.39		234.74
	1723	ND2	ASN A ASN A			23.362	9.32 9.83	_	234.74
-0	1724	C	ASN A	2	7 11.425	22.453 24.569	9.07		249.69
50) 1725 1726	Ň	GLY A	. 2	8 11.267		9.38	ю 1.00	249.69
	1727	CA	GLY A	2			8.76		249.69 249.69
	1728	C	GLY A		28 12.886 28 12.749	26.475	7.55		249.69
	1729	0 N	ASN A	-	9 13.240	27.275	9.60 9.12		∔9.69
55	5 1730 1731	CA	ASN	A, ?	29 13.468		10.3	21 1.00	249.69
	1732	CB	ASN		29 13.452 29 13.40°		9.8		249.69 249.69
	1733	CG	ASN	• •	29 13.40° 29 13.22°		8.7		249.69
	1734	OD1			29 13.54	8 31.993	10.8 8.3		249.69
6	0 1735	ND2 C	ASN	• •	29 14.76			90 1.00	249.69
	1736 1737	Ö	ASN	A	29 14.72			61 1.00	249.69
	1737	N	ASN		30 15.89 30 17.15		8.1	1.00	
	1739	CA	ASN		30 17.15 30 18.00	2 29.581	•	395 1.00 911 1.00	
6	55 1740		ASN ASN		30 17.34	₁₉ 30.959	•	911 1.00 960 1.00	0.40.00
	1741				30 17.26		-	744 1.00) 249.69
	1742 1743		2 ASN	A	30 16.8		·	919 1.00	249.69
	1744	C	ASN	A	30 17.99 30 18.1			774 1.00	249.69
	70 1745		ASN	Α.					

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						- 04	969	8.987	1.00	249.69
		N	PHE A	31	18.51	-	3.668 5.474	8.836	1.00	249.69
	746	CA	PHE A	31	19.34	~ _	5.733	9.416	1.00	249.69
	747 748	CB-	PHE A	31	20.74	~ ~	6.957	8.841	1.00	249.69 249.69
	748 749	ÇG.	PHE A	31	21.42		8.234	9.300	1.00	249.69
	750	CD1	PHE A	31	22.3		6.835	7.822	1.00 1.00	249.69
	751	CD2	PHE A	31 31	21.7	06 2	9.372	8.749	1.00	249.69
	752	CE1	PHE A	31	22.9	78 2	27.971	7.263 7.730	1.00	249.69
1	1753	CE2	PHE A	31	22.6	•	29.238	9.450	1.00	249.69
	1754	CZ	PHE A	31	18.7	JE -	24.200 24.144	10.647	1.00	249.69
	1755	C	PHE A	31	18.4	~~	23.175	8.608	1.00	249.69
	1756	N	PHE A	32	18.6	~~	21.879	9.017	1.00	249.69 249.69
	1757 1758	CA	PHE A	32	18.0 16.7	1 72	21.579	8.201	1.00 1.00	249.69
	1759	СВ	PHE A	32 32	15.9		20.469	8.766	1.00	249.69
15	1760	CG	PHE A PHE A	32	15.		20.621	9.991 8.0 64	1.00	249.69
	1761	CD1	PHE A PHE A	32	15.		19.274	10.509	1.00	249.69
	1762	CD2	PHE A	32		496	19.598 18. 24 5	8.573	1.00	249.69
	1763	CE1 CE2	PHE A	32		990	18.408	9.798	1.00	249.69
00	1764	CZ	PHE A	32		345	20.757	8.821	1.00	249.69 249.69
20	1765 1766	č	PHE A	32		.088 .125	20.964	8.170	1.00	231.29
	1767	Ö	PHE A	32		.798	19.569	9.358	1.00 1.00	231.29
	1768	N	GLU A	33 33		.741	18.455	9.270	1.00	249.69
	1769	CA	GLU A	33	20	.145	18.036	10.688 10.751	1.00	249.69
25	1770	CB	GLU A	33	21	.430	17.234	9.925	1.00	249.69
	1771	CD	GLU A	33		2,544	17.870 19.095	10.061	1.00	249.69
	1772	OE1	GLU A	33		2.781	17.142	9.140	1.00	249.69 231.29
	1773	OE2	GLU A	33		3.193 9.334	17.212	8.477	1.00	231.29
30	1774 1775	Č	GLU A	33	_	0.088	16.746	7.624	1.00 1.00	249.69
30	1776	0	GLU A	33 34		8.156	16.671	8.765 8.096	1.00	249.69
	1777	N	VAL A	34		7.677	15.462	8.664	1.00	206.86
	1778	CA	VAL A	34	, 1	6.288	15.045	8.012	1.00	206.86
	1779	CB CG1	VAL A	34		5.809	13.765 14.858	10.166	1.00	206.86
35	1780	CG2	VAL A		•	6.382	15.536	6.560	1.00	249.69 249.69
	1781 1782	Č	VAL A		•	17.599 17.381	16.608	5.977		249.69
	1783	Ö	VAL A	_	•	17.793	14.378	5.920		-40.00
	1784	N	SER A			17.744	14.245	4.458		4-7-40
40	1785	CA	SER A	•		18.968	13.478	3.941 4.268		177.13
•	1786	CB	SER A	•	35	18.874	12.099	4.082		249.69
	1787	og C	SER		35	16.483	13.467 13.245	2.90	2 1.00	249.69 238.60
	1788	ŏ	SER	Α :	35	16.208	13.038	5.10		
45	1789 1790	Ň	SER	•	36	15.739 14.506	12.290	4.90	2 1.00 2 1.00	
45	1791	CA	SER		36 36	14.437	11.091	5.86		-10.00
	1792	CB	SER SER		36	14.205	11.498	7.20 5.12		0 238.60
	1793	og.	SER	Â	36	13.298	13.200	6.23		o 238.60
-	1794	C	SER		36	12.807	13.368 13.795	4.03	30 1.0	
50	0 1795	Ň	THR		37	12.835 11.686	14,678	4.00		
	1796 1797	CA	THR		37	12.108	16.135	3.7		
	1798	CB	THR		37 37	13.071	16.572	4.73 3.7		n 216.59
	1799	001			37	10.904	17.061	3.7	••	00 223.58
5	5 1800	CG2	THR	Â	37	10.706	14.165	1.9	• •	00 223.58
	1801	C	THR		37	11.104	13.773 14.148	3.3	1.1	00 249.69
	1802	Ň	LYS	Α	38	9.425	13.655	2.4		00 249.69 00 249.69
	1803 1804		LYS	Α	38	8.410 7.490	12.670			242.00
	50 1805		LYS	Ą	38 38	8.232	11.473			.00 249.69 .00 249.69
•	1806	CG			38	7.296	10.511			.00 249.69
	1807	CD		Α .	38	8.060	9.293			.00 249.69
	1808	S CE) A	38	7.181	8.326			no 249.69
	1809			Â	38	7.588	14.782 15.793		456 1	1.00 249.69
	65 1810			s A	38	7.301	14.611	0	.536 1	1.00 201.19 1.00 201.19
	1811 1811	•		PA	39	7.229 6.425			• • • •	470.40
	181	3 C/		PA	39 39	7.256				450 40
	181	4 CI		P A	39	8.384		-0	.741	1.00 1/3.48
	70 181		G IH	r ^	-					

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	1816	CD2	TRP A	39	8.282	18.328	0.122	1.00	173.49
	1817	CE2	TRP A	39	9.574	18.892	0.223	1.00	173.49
	1818	CE3	TRP A	39	7.223	18.950	0.812	1.00	173.49
_	1819	CD1	TRP A	39	9.703	17.079	-1.099	1.00	173.49
5	1820	NE1	TRP A	39	10.418 9.836	18.112 20.031	-0.528 0.972	1.00 1.00	173.49 173.49
	1821	CZ2	TRP A	39 39	7.489	20.083	1.554	1.00	173.49
	1822 1823	CZ3 CH2	TRP A	39	8.785	20.611	1.629	1.00	173.49
	1824	C	TRP A	39	5.263	14.870	-0.821	1.00	201.19
10	1825	ŏ	TRP A	39	5.473	13.844	-1.463	1.00	201.19
	1826	N	PHE A	40	4.045	15.385	-0.655	1.00	233.06
	1827	CA	PHE A	40	2.875	14.733	-1.231	1.00	233.06
	1828	СВ	PHE A	40	1.983	14.154	-0.122	1.00	249.42
. ~	1829	CG	PHE A	40	2.671	13.151	0.775 1.820	1.00 1.00	249.42 249.42
15	1830	CD1	PHE A	40	3.484 2.482	13.580 11.778	0.592	1.00	249.42 249.42
	1831	CD2	PHE A PHE A	40 40	2.462 4.098	12.658	2.674	1.00	249.42
	1832 1833	CE1 CE2	PHE A	40	3.089	10.854	1.435	1.00	249.42
	1834	CZ	PHE A	40	3.899	11.294	2.479	1.00	249.42
20	1835	č	PHE A	40	2.023	15.621	-2.139	1.00	233.06
	1836	Ó	PHE A	40	0.945	16.063	-1.744	1.00	233.06
	1837	N	HIS A	41	2.506	15.858	-3.358	1.00	146.58
	1838	ÇA	HIS A	41	1.787	16.676	-4.340	1.00	146.58
	1839	CB	HIS A	41	2.663	16.905	-5.569	1.00	196.00
25	1840	CG	HIS A	41	2.012	17.747	-6.619 -7.971	1.00 1.00	196.00 196.00
	1841	CD2	HIS A	41 41	2.035 1.259	17.661 18.864	-6.322	1.00	196.00
	1842 1843	ND1 CE1	HIS A HIS A	41	0.849	19.429	-7.441	1.00	196.00
	1844	NE2	HIS A	41	1.308	18.719	-8.457	1.00	196.00
30	1845	C	HIS A	41	0.459	16.041	-4.776	1.00	146.58
50	1846	ŏ	HIS A	41	0.458	15.095	-5.564	1.00	146.58
	1847	N	ASN A	42	-0.660	16.586	-4.280	1.00	208.40
	1848	CA	ASN A	42	-2.004	16.067	-4.570	1.00	208.40
	1849	CB	ASN A	42	-2.229	15.933	-6.087	1.00	249.69
35	1850	CG	ASN A	42	-2.538	17.270 18.251	-6.7 63 -6.553	1.00 1.00	249.69 249.69
	1851	OD1 ND2	ASN A ASN A	42 42	-1.824 -3.591	17.305	-7.583	1.00	249.69
	1852 1853	C	ASN A	42	-2.173	14.703	-3.887	1.00	208.40
	1854	ŏ	ASN A	42	-2.981	13.871	-4.302	1.00	208.40
40	1855	Ň	GLY A	43	-1.401	14.499	-2.824	1.00	249.69
	1856	CA	GLY A	43	-1.445	13.248	-2.092	1.00	249.69
	1857	С	GLY A	43	-0.354	12.288	-2.555	1.00	249.69
	1858	0	GLY A	43	0.302	11.620	-1.744	1.00	249.69
45	1859	N	SER A	44	-0.158	12.222 11.350	-3.870 -4.481	1.00 1.00	243.81 243.81
45	4860	CA	SER A SER A	44 44	0.845 0.812	11.493	-6.004	1.00	249.09
	1861 1862	CB OG	SER A	44	-0.450	11.141	-6.535	1.00	249.69
	1863	c	SER A	44	2.250	11.676	-4.002	1.00	243.81
	1864	ŏ	SER A	44	2.714	12.806	-4.162	1.00	243.81
50	1865	Ň	LEU A	45	2.936	10.687	-3.437	1.00	249.69
	1866	CA	LEU A	45	4.294	10.912	-2.958	1.00	249.69
	1867	CB	LEU A	45	4.913	9.605	-2.458	1.00	240.25
	1868	CG	LEU A	45	6.324	9.745	-1.879	1.00	240.25 240.25
66	1069	CD1	LEU A	45	6.328	10.787 8.405	-0.773 -1.351	1.00 1.00	240.25 240.25
55	1870	CD2	LEU A LEU A	45 45	6. 798 5.1 6 0	11.512	-4.070	1.00	248.09
	1871 1872	C	LEU A	45	4.939	11.248	-5.256	1.00	249.69
	1873	Ň	SER A	46	6.136	12.329	-3.675	1.00	216.07
	1874	CA	SER A	46	7.028	12.988	-4.621	1.00	216.07
60	1875	СВ	SER A	46	7.156	14.473	-4.270	1.00	249.69
	1876	OG	SER A	46	7.934	15.159	-5.237	1.00	249.69
	1877	C	SER A	46	8.409	12.344	-4.645	1.00	216.07
	1878	0	SER A	46	8.733	11.515	-3.795	1.00	216.07
65	1879	N	GLU A	47	9.223	12.753	-5.616	1.00	204.74 204.74
65	1880	CA	GLU A	47	10.572	12.214 12.162	-5.797 -7.289	1.00 1.00	249.69
	1881	CB	GLU A GLU A	47 47	10.901 9.973	11.256	-8.078	1.00	249.69
	1882 1883	CD	GLU A	47	10.299	11.239	-9.554	1.00	249.69
	1884	OE1	GLU A	47	10.185	12.307	-10.203	1.00	249.69
70	1885	OE2	GLU A	47	10.673	10.158	-10.066	1.00	249.69

	1886	С	O111 A	4-	44 700	40.000			
	1887	ŏ	GLU A GLU A	47	11.702	12.933	-5.059	1.00	204.74
	1888	N:	GLU A	47	12.819	12.424	-4.995	1.00	204.74
	1889	CA	GLU A	48 48	11.429 12.459	14.113 14.833	-4.512	1.00	206.77
5	1890	CB	GLU A	48	12.439	16.344	-3.780	1.00	206.77
•	1891	CG	GLU A	48	13.200	17.159	-3.812 -2.982	1.00	249.43
	1892	CD	GLU A	48	14.627	17.139	-2.962 -3.507	1.00	249.43
	1893	OE1	GLU A	48	14.902	17.685	-3.507 -4.569	1.00	249.43
	1894	OE2	GLU A	48	15.472	16.431	-2.859	1.00	249.43
10	1895	Č	GLU A	48	12.492	14.344	-2.335 -2.335	1.00 1.00	249.43
	1896	Ō	GLU A	48	11.500	13.825	-1.811	1.00	206.77
	1897	N	THR A	49	13.648	14.506	-1.702	1.00	206.77
	1898	CA	THR A	49	13.844	14.085	-0.324	1.00	249.69 249.69
	1899	CB	THR A	49	14.806	12.890	-0.252	1.00	249.53
15	1900	OG1	THR A	49	16.030	13.218	-0.928	1.00	249.53
	1901	CG2	THR A	49	14.174	11.671	-0.909	1.00	249.53
	1902	С	THR A	49	14.417	15.232	0.500	1.00	249.69
	1903	0	THR A	49	14.224	15.294	1.716	1.00	249.69
20	1904	N	ASN A	50	15.128	16.136	-0.166	1.00	249.69
20	1905	, CA	ASN A	50	15.710	17.294	0.504	1.00	249.69
	1906	CB	ASN A	50	16.438	18.174	-0.519	1.00	232.42
	1907	CG	ASN A	50	17.276	19.254	0.134	1.00	232.42
	1908	OD1	ASN A	50	17.063	19.590	1.301	1.00	232.42
25	1909	ND2	ASN A	50	18.219	19.813	-0.615	1.00	232.42
23	1910	C	ASN A	50	14.552	18.073	1.142	1.00	249.69
	1911	0	ASN A	50	13.423	18.003	0.658	1.00	249.69
	1912	N	SER A	51	14.817	18.808	2.217	1.00	181.87
	1913	CA	SER A	51	13.759	19.568	2.873	1.00	181.87
30	1914	CB	SER A	51	14.240	20.110	4.220	1.00	249.47
30	1915	oe	SER A	51	15.152	21.181	4.047	1.00	249.47
	1916 1917	C	SER A	51	13.249	20.725	2.016	1.00	181.87
	1918	N	SER A SER A	51 50	12.180	21.269	2.293	1.00	181.87
	1919	CA	SER A	52 52	14.007	21.104	0.984	1.00	193.91
35	1920	ČŠ	SER A	52 52	13.606 14.735	22.199 23.217	0.087	1.00	193.91
-	1921	og	SER A	52	15.064	23.831	-0.086	1.00	144.08
	1922	č	SER A	52	13.196	21.706	1.139 -1.297	1.00	144.08
	1923	ŏ	SER A	52	14.045	21.765	-1.287 -2.126	1.00 1.00	193.91
	1924	Ň	LEU A	53	11.890	21.680	-1.539	1.00	193.91 177.42
40	1925	CA	LEU A	53	11.346	21.239	-2.817	1.00	177.42
	1926	СВ	LEU A	53	10.034	20.488	-2.595	1.00	145.45
	1927	CG	LEU A	53	9.082	20.340	-3.785	1.00	145.45
	1928	CD1	LEU A	. 53	9.821	19.891	-5.043	1.00	145.45
	1929	CD2	LEU A	53	7.997	19.343	-3.401	1.00	145.45
45	1930	C	LEU A	53	11.108	22.423	-3.737	1.00	177.42
	1931	0	LEU A	53	10.143	23.168	-3.574	1.00	177.42
	1932	N	ASN A	54	11.991	22.591	-4.709	1.00	220.39
	1933	CA	ASN A	54	11.845	23.692	-5.63 5	1.00	220.39
50	1934	CB	ASN A	54	13.187	24.045	-6.254	1.00	193.36
30	1935	CG	ASN A	54	14.109	24.677	-5.264	1.00	193.36
	1936	OD1	ASN A	54	13.746	25.644	-4.602	1.00	193.36
	1937 1938	ND2 C	ASN A ASN A	54	15.311	24.140	-5.145	1.00	193.36
	1939	ŏ		54	10.834	23.415	-6.729	1.00	220.39
55	1940	Ñ	ASN A ILE A	54 55	10.486	22.267	-7.009	1.00	220.39
55	1941	ČA	ILE A	55 55	10.362	24.496	-7.333	1.00	206.48
	1942	ČB	ILE A	55 55	9.393 7.984	24.451 24.867	-8.415 7.001	1.00	206.48
	1943	CG2	ILE A	55	7.135	25.353	-7.921	1.00	168.43
	1944	CG1	ILE A	55	7.316	23.696	-9.080 -7.206	1.00	168.43
60	1945	CD1	ILE A	55 55	5.920	24.004	-7.206 -6.681	1.00 1.00	168.43
_	1946	C	ILE A	55	9.877	25.442	-9.459	1.00	168.43
	1947	ō	ILE A	55	9.979	26.641	-9.459 -9.190	1.00	206.48 206.48
	1948	Ň	VAL A	56	10.194	24.943	-10.646	1.00	242. 7 7
	1949	CA	VAL A	56	10.667	25.821	-11.700	1.00	242.77
65	1950	CB	VAL A	56	11.790	25.165	-12.499	1.00	249.69
	1951	CG1	VAL A	56	12.589	26.233	-13.240	1.00	249.69
	1952	CG2	VAL A	56	12.687	24.377	-11.562	1.00	249.69
	1953	Ç	VAL A	56	9.511	26.168	-12.624	1.00	242.77
70	1954	0	VAL. A	56	8.354	26.060	-12.225	1.00	242,77
70	1955	N	ASN A	57	9.822	26.580	-13.853	1.00	177.18
									• =

1	956 1957 1958 1959	CA CB CG. OD1	ASN A ASN A ASN A	57	8.804 9.265 10.430 10.372	26.971 26.619 27.489 28.721 26.853	-14.835 -16.250 -16.705 -16.617 -17.187	1.00 1.00 1.00 1.00 1.00	177.18 249.69 249.69 249.69 249.69
5	1960 1961 1962 1963	ND2 C O N	ASN A ASN A ASN A ALA A	57 57 57 58 58	11.494 7.436 7.105 6.661 5.322	26.374 25.264 27.166 26.838	-14.547 -14.964 -13.816 -13.362	1.00 1.00 1.00 1.00 1.00	177.18 177.18 241.59 241.59 177.10
10	1964 1965 1966 1967 1968	CA CB C O N	ALA A ALA A ALA A LYS A	58 58 58 59	4.739 4.339 3.857 4.031	28.038 26.363 27.134 25.077 24.446	-12,623 -14,416 -15,237 -14,363 -15,277	1.00 1.00 1.00 1.00	241.59 241.59 126.26 126.26
15	1969 1970 1971 1972	CA CB CG CD	LYS A LYS A LYS A LYS A LYS A	59 59 59 59	3.078 3.620 4.959 5.515 6.883	23.088 23.183 21.808 21.939	-15.761 -16.494 -16.859 -17.528	1.00 1.00 1.00 1.00 1.00	249.69 249.69 249.69 249.69 249.69
20	1973 1974 1975 1976 1977	CE NZ C O N	LYS A LYS A LYS A PHE A	59 59 59 60	7.458 1.790 1.810 0.672	20.619 24.246 23.891 24.490 24.356	-17.910 -14.486 -13.311 -15.139 -14.497	1.00 1.00 1.00 1.00	126.26 126.26 178.77 178.77
25	1978 1979 1980 1981	CA CB CG CD1	PHE A PHE A PHE A PHE A PHE A	60 60 60 60	-0.622 -1.715 -1.824 -2.296 -1.468	24.325 25.601 25.585 26.820	-15.570 -16.362 -17.670 -15.794	1.00 1.00 1.00 1.00 1.00	238.68 238.68 238.68 238.68 238.68
30	1982 1983 1984 1985 1986	CD2 CE1 CE2 CZ C	PHE A PHE A PHE A PHE A	60 60 60	-2.411 -1.580 -2.053 -0.746 -1.468	26.758 28.002 27.969 23.132 23.162	-18.400 -16.515 -17.821 -13.592 -12.588	1.00 1.00 1.00 1.00	238.68 238.68 178.77 178.77
35	1987 1988 1989 19 9 0	O N CA CB	PHE A GLU A GLU A GLU A	60 61 61 61 61	-0.040 -0.076 0.665 0.091	22.063 20.822 19.719 19.402	-13.948 -13.181 -13.945 -15.330 -16.264	1.00 1.00 1.00 1.00 1.00	249.03 249.03 249.30 249.30 249.30
40	1991 1992 1993 1994 1995	CG CD OE1 OE2 C	GLU A GLU A GLU A	61 61 61 61	0.076 1.132 -0.997 0.537	20.605 21.254 20.895 20.991 20.236	-16.254 -16.436 -16.833 -11.792 -10.870	1.00 1.00 1.00 1.00	249.30 249.30 249.03 249.03
	1996 1997 1998 1999	O N CA CB	GLU A ASP A ASP A	61 62 62 62 62	0.222 1.412 2.062 3.191 4.167	21.984 22.251 23.264 22.856	-11.648 -10.372 -10.539 -11.598	1.00 1.00 1.00 1.00	157.91 157.91 172.18 172.18 172.18
45	2001 2002 2003	CG OD1 OD2 C	ASP A ASP A ASP A ASP A	62 62 62 2	4.368 4.743 1.058 1.266	21.633 23.753 22.795 22.700	-11.779 -12.244 -9.366 -8.159 -9.864	1.00	172.18 157.91 157.91 191.12
50	2004) 2005 2006 2007 2008	N CA CB OG	SER A SER A SER A	63 63 63	-1.061 -2.179 -1.685	23.384 23.933 24.576 25.593 22.778	-8.991 -9.822 -10.671 -8.186	1.00 1.00 1.00 1.00	191.12 203.60 203.60 191.12
5	2009 5 2010 2011 2012	C O N CA	SER A SER A GLY A GLY A	63 64 6	-2.040 4 -1.662 4 -2.199	21.773 22.907 21.821 21.897	-8.75 -6.87 -6.08 -4.59 -4.06	1.00 7 1.00 6 1.00	191.12 195.42 195.42 195.42 195.42
6	2013 2014 50 2015 2016 2017	C O N CA CB	GLU A GLU A GLY A	6 6	4 -1.583 5 -2.199 5 -2.064 5 -3.302	22.940 20.765 20.613 19.876 19.481	-3.93 -2.48 -1.96 -0.51	3 1.00 4 1.00 59 1.00	249.69 249.69 246.11 246.11
(2018 2019 55 2020 2021	CG CD OE1 OE2	g GLU	A 6	55 -3.277 55 -4.310 55 -4.201 55 -5.230 65 -0.790	18.417 17.309 18.684	-0.20 -0.7 0.5 -2.1	79 1.00 97 1.00 12 1.00	246.11 246.11 246.11 249.69 249.69
	2022 2023 2024 70 2025	. N	GLU GLU TYR TYR	A (65 -0.613 66 0.083 66 1.334	18.711 20.456	-2.5 -1.3 -0.8	08 1.00	196.27

	2026 2027	CB CG	TYR A	66	2.534	20.641	-1.324	1.00	181.47
	2027	CD ₁	TYR A TYR A	66 66	2.737	20.798	-2.807	1.00	181.47
	2029	CET	TYR A	66	1.966 2.227	21.687 21.911	-3.549	1.00	181.47
5	2030	CD2	TYR A	66	3.769	20.122	-4.896 -3.454	1.00 1.00	181.47
	2031	CE2	TYR A	66	4.040	20.332	-4.800	1.00	181.47 181.47
	2032	CZ	TYR A	66	3.268	21.230	-5.513	1.00	181.47
	2033	ОН	TYR A	66	3.561	21.460	-6.838	1.00	181.47
10	2034 2035	C	TYR A TYR A	66	1.462	19.616	0.622	1.00	196.27
10	2036	Ň	TYR A LYS A	66 67	0.665 2.493	20.149	1.402	1.00	196.27
	2037	ČA	LYS A	67	2.778	18.862 18.572	1.021 2.435	1.00	214.47
	2038	СВ	LYS A	67	1.630	17.783	3.059	1.00 1.00	214.47
س .	2039	CG	LYS A	67	1.262	16.527	2.300	1.00	179.29 179.29
15	2040	CD	LYS A	67	0.071	15.859	2.955	1.00	179.29
	2041 2042	CE NZ	LYS A	67	-0.626	14.887	2.008	1.00	179.29
	2042	C	LYS A LYS A	67 67	-1.808 4.077	14.194	2.632	1.00	179.29
	2044	ŏ	LYS A	67	4.546	17.799 17.060	2.681 1.826	1.00	214.47
20	2045	N	CYS A	68	4.644	17.981	3.869	1.00 1.00	214.47 202.66
	2046	CA	CYS A	68	5.865	17.291	4.259	1.00	202.66
	2047	C	CYS A	68	5.713	16.618	5.621	1.00	202.66
	2048 2049	O CB	CYS A	68	4.961	17.075	6.483	1.00	202.66
25	2050	SG	CYS A CYS A	68 68	7.067	18.245	4.273	1.00	195.74
	2051	N	GLN A	69	7.101 6.439	19.551 15.519	5.556	1.00	195.74
	2052	CA	GLN A	69	6.420	14.730	5.797 7.024	1.00 1.00	233.18
	2053	CB	GLN A	69	5.367	13.631	6.896	1.00	233.18 249.69
20	2054	CG	GLN A	69	5.562	12.460	7.835	1.00	249.69
30	2055	CD	GLN A	69	4.580	11.333	7.569	1.00	249.69
	2056 2057	OE1 NE2	GLN A GLN A	69	4.451	10.865	6.436	1.00	249.69
	2058	C	GLN A	69 69	3.888 7. 7 98	10.885	8.615	1.00	249.69
	2059	ŏ	GLN A	69	8.485	14.111 13.796	7.224 6.254	1.00 1.00	233.18
35	2060	N	HIS A	70	8.206	13.942	8.477	1.00	233.18 249.54
	2061	CA	HIS A	70	9.508	13.348	8.757	1.00	249.54
	2062	CB	HIS A	70	10.202	14.086	9.904	1.00	249.69
	2063 2064	CG CD2	HIS A HIS A	70	10.674	15.458	9.536	1.00	249.69
40	2065	ND1	HIS A	70 70	10.459 11.475	16.662 15.699	10.116	1.00	249.69
	2066	CE1	HIS A	70	11.731	16.992	8.439 8.359	1.00 1.00	249.69
	2067	NE2	HIS A	70	11.126	17.600	9.366	1.00	249.69 249.69
	2068	Ç	HIS A	70	9.393	11.867	9.084	1.00	249.54
45	2069 2070	0	HIS A	70	8.327	11.270	8.917	1.00	249.54
73	2070	N CA	GLN A GLN A	71 71	10.496	11.283	9.549	1.00	249.69
	2072	CB	GLN A	71	10.546 11.944	9. 863 9.520	9.894	1.00	249.69
	2073	CG	GLN A	71	12.318	8.033	10.429 10.415	1.00 1.00	249.69 249.69
50	2074	CD	GLN A	71	12.356	7.432	9.015	1.00	249.69 249.69
50	2075	OE1	GLN A	71	12.933	8.009	8.090	1.00	249.69
	2076 2077	NE2	GLN A	71	11.749	6.257	8.859	1.00	249.69
	2078	CO	GLN A GLN A	71 71	9.474	9.485	10.925	1.00	249.69
	2079	Ň	GLN A	72	8.737 9.383	8. 50 5 10. 27 0	10.747	1.00	249.69
55	2080	CA	GLN A	72	8.413	10.270	11.995 13.056	1.00 1.00	249.69
	2081	CB	GLN A	72	9.148	9.484	14.292	1.00	249.69 249.69
	2082	CG	GLN A	72	8.266	9.132	15.487	1.00	249.69
	2083 2084	CD	GLN A	72	9.085	8.768	16.717	1.00	249.69
60	2085	OE1 NE2	GLN A GLN A	72	9.910	7.853	16.679	1.00	249.69
-	2086	C	GLN A	72 72	8.860 7.634	9.486 11.288	17.817	1.00	249.69
	2087	Ö	GLN A	72	7.602	11.722	13.402 14.558	1.00 1.00	249.69
	2088	N	VAL A	73	7.011	11.891	12.393	1.00	249.69 249.69
C E	2089	CA	VAL A	73	6.233	13.108	12.595	1.00	249.69
65	2090	CB	VAL A	73	7.036	14.377	12.200	1.00	239.35
	2091 2092	CG1 CG2	VAL A	73 72	6.321	15.615	12.720	1.00	239.35
	2092	C	VAL A VAL A	73 73	8.449 4.979	14.304	12.750	1.00	239.35
	2094	ŏ	VAL A	73 73	4.979 5.014	13.047 12.526	11.731 10.619	1.00	249.69
70	2095	N	ASN A	74	3.875	13.578	12.245	1.00 1.00	249.69 249.69
									2 70.00

	2096 2097 2098 2099	CA CB CQ OD1 ND2	ASN A ASN A	74 74 74 74 74	2.627 1.448 1.421 1.672 1.112	13.580 13.799 12.775 11.588 13.230	11.494 12.450 13.581 13.354 14.793 10.404	1.00 1.00 1.00 1.00 1.00	249.69 244.75 244.75 244.75 244.75 249.69
_	2100 2101 2102 2103	002	ASN A ASN A GLU A GLU A	74 74 75 75	2.667 2.979 2.362 2.370	14.663 15.828 14.262 15.160	10.680 9.167 8.008	1.00 1.00 1.00	249.69 249.69 249.69 249.69
10	2104 2105 2106 2107	CA CB CG CD	GLU A GLU A GLU A GLU A	75 75 75 75 75	1.656 0.447 -0.086 0.722	14.485 13.641 12.806 12.115	6.826 7.216 6.064 5.408	1.00 1.00 1.00 1.00	249.69 249.69 249.69 249.69
15	2108 2109 2110 2111	OE1 OE2 C	GLU A GLU A GLU A	75 75 75 75 76	-1.312 1.786 0.776 2.437	12.831 16.556 16.714 17.562	5.820 8.262 8.954 7.682	1.00 1.00 1.00 1.00	249.69 249.69 249.69 249.69
20	2112 2113 2114 2115	N CA CB OG	SER A SER A SER A	76 76 76 76 76	2.037 3.093 3.026 0.691	18.959 19.877 19.838 19.291	7.833 7.212 5.796 7.206	1.00 1.00 1.00 1.00	185.73 185.73 249.69 249.69
	2116 2117 2118 2119	C O N CA	SER A SER A GLU A	76 77 77 77	0.212 0.093 -1.187 -1.695	18.589 20.382 20.845 22.053	6.316 7.677 7.153 7.952	1.00 1.00 1.00 1.00	249.69 249.69 249.63
25	2120 2121 2122 2123	CB CG CD OE1	GLU A GLU A GLU A	77 77 77	-2.038 -3.175 -3.606 -3.633	21.734 20.742 20.194 20.508	9.394 9.515 8.477 10.653	1.00 1.00 1.00 1.00	249.63 249.63 249.63 249.63
30	2124 2125 2126 2127	OE2 C O N	GLU A GLU A GLU A PRO A	77 77 77 78	-0.961 -0.262 -1.556 -2.599	21,250 22,226 20,502 19,491	5.701 5.423 4.757 4.999	1.00 1.00 1.00 1.00	249.69 249.69 227.00 247.88
35	2128 2129 2130 2131	CD CA CB CG	PRO A PRO A PRO A	78 78 78 78	-1.413 -2.583 -2.752 -1.488	20.781 20.012 18.854 22.271	3.321 2.710 3.641 2.998	1.00 1.00 1.00 1.00	227.00 247.88 247.88 227.00
40	2132 2133 2134 2135	C O N CA	PRO A PRO A VAL A VAL A	78 78 79 79	-2.039 -0.910 -0.966 0.390	23.054 22.665 24.059 24.785	3.771 1.871 1.435 1.549	1.00 1.00 1.00 1.00	227.00 169.93 169.93 154.03
-10	2136 2137 2138 2139	CB CG1 CG2 C	VAL A VAL A VAL A VAL A	79 79 79 79	0.329 0.721 -1.342 -0.883	26.125 25.022 23.987 23.087	0.825 3.014 -0.017 -0.710	1.00 1.00 1.00 1.00	154.03 154.03 169.93 169.93
45	2140 2141 2142 2143	O N CA CB	VAL A TYR A TYR A TYR A	79 80 80 80	-2.175 -2.581 -4.096 -4.606	24.911 24.874 25.028 24.573	-0.487 -1.888 -2.025 -3.372	1.00 1.00 1.00 1.00	161.75 161.75 221.72 221.72
50	2144	CG CD1 CE1 CD2	TYR A TYR A TYR A TYR A	80 80 80	-4.874 -5.296 -4.773	23.227 22.792 25.478 25.052	-3.618 -4.874 -4.418 -5.679	1.00 1.00 1.00	221.72 221.72 221.72 221.72
5	2148 2149 5 2150 2151	CE2 CZ OH C	TYR A TYR A TYR A TYR A TYR A	80 80 80 80	-5.193 -5.451 -5.860 -1.895 -1.812	23.708 - 23.276 - 25.939 - 27.096	-5.896 -7.134 -2.725 -2.329	1.00 1.00 1.00 1.00	221.72 221.72 161.75 161.75 159.92
6	2152 2153 2154 60 2155	O N CA CB CG	LEU A LEU A LEU A	81 81 81	1,353	25.534 26.451 25.951 26.823	-3.889 -4.789 -5.13 -6.18 -5.60	9 1.00 8 1.00 8 1.00	159.92 117.26 117.26 117.26
	2156 2157 2158 2159	CD1 CD2 C	LEU A LEU A LEU A	81 81	2.692 -1.550	28.213 26.221 26.562 25.541	-6.60 -6.06 -6.67 -6.47	0 1.00 7 1.00 8 1.00	117.26 159.92 159.92 176.90
(55 2160 2161 2162 2163	N CA CB CG	GLU / GLU / GLU /	A 82 A 83 A 83	2 -1.879 2 -2.637 2 -3.950	27.786 27.978 28.697 28.382	-0.47 -7.70 -7.42 -8.45 -8.10	09 1.00 27 1.00 54 1.00	176.90 239.33 239.33 239.33
	70 2165	CD	GLU	-		29.072	-6.10		

	2166	OE1 OE2	GLU A		-6.678 -7.038	29.235 29.437	-6.970 -9.139 -8.720	1.00 1.00 1.00	239.33 239.33 176.90
	2167 2168	č	GLU A	82	-1.815	28.772	-8.369	1.00	176.90
	2169	Ö	GLU A	82	-1.176	29.768 28.315	-9.973	1.00	167.08
	2170	N	VAL A	83	-1.818	28.988	-11.050	1.00	167.08
J ,	2171	CA	VAL A	83	-1.078 -0.163	28.034	-11.817	1.00	127.07
	2172	CB	VAL A	83	0.595	28.807	-12.899	1.00	127.07
	2173	CG1	VAL A	83 83	0.800	27.368	-10.847	1.00	127.07
	2174	CG2	VAL A	83	-2.036	29.634	-12.043	1.00	167.08
10	2175	Ç	VAL A VAL A	83	-3.077	29.071	-12.390	1.00	167.08
	2176	0	PHE A	84	-1.653	30.810	-12.524	1.00 1.00	136.71 136.71
	2177	N CA	PHE A	84	-2.502	31.588	-13.412	1.00	180.02
	2178	CB	PHE A	84	-3.039	32.805	-12.669	1.00	180.02
15	2179	ÇG	PHE A	84	-3.878	32.481	-11.481 -10.263	1.00	180.02
13	2180 2181	CD1	PHE A	84	-3.296	32.143	-11.575	1.00	180.02
	2182	CD2	PHE A	84	-5.259	32.534 31.871	-9.157	1.00	180.02
	2183	CE'	PHE A	84	-4.085	32.266	-10.484	1.00	180.02
	2184	CE2	PHE A	84	-6.055 -5,471	31.933	-9.274	1.00	180.02
20	2185	CZ	PHE A	84	-1.917	32.125	-14.692	1.00	136.71
	2186	Ç	PHE A	84 84	-0.710	32.289	-14.838	1.00	136.71
	2187	0	PHE A	85	-2.822	32.440	-15.606	1.00	185.25
	2188	N	SER A SER A	85	-2.470	33.050	-16.871	1.00	185.25 191.52
	2189	CA	SER A	85	-2.639	32.088	-18.036	1.00	191.52
25	2190	CB	SER A	85	-2.269	32.736	-19.246	1.00	185.25
	2191	C OG	SER A	85	-3.462	34.193	-17.012	1.00 1.00	185.25
	2192	ŏ	SER A	85	-4.680	33.960	-17.105 -17.002	1.00	167.09
	2193 2194	Ň	ASP A	86	-2.940	35.422	-17.117	1.00	167.09
30	2195	ČA	ASP A	86	-3.769	36.623 36.701	-15.951	1.00	156.75
20	2196	СВ	ASP A	86	-4.744	37.252	-16.358	1.00	156.75
	2197	CG	ASP A	86	-6.072	38.341	-16.985	1.00	156.75
	2198	OD1	ASP A	86	-6.110 -7.083	36.587	-16.045	1.00	156.75
	2199	OD2	ASP A	86 86	-2.888	37.852	-17.101	1.00	167.09
35	2200	Ç	ASP A ASP A	86	-1.708	37.760	-16.775	1.00	167.09 147.13
	2201	0	TRP A	87	-3.455	39.005	-17.438	1.00	147.13
	2202	N	TRP A	87	-2.665	40.233	-17.435	1.00 1.00	200.84
	2203	CA CB	TRP A	87	-3.446	41.371	-18.079	1.00	200.84
40	2204	CG	TRP A	87	-3.221	41.441	-19.553 -20.563	1.00	200.84
40	2205 2206	CD2	TRP A	87	-4.022	40.824	-21.798	1.00	200.84
	2207	CE2	TRP A	87	-3.413	41.103 40.061	-20.542	1.00	200.84
	2208	CE3	TRP A	87	-5.199	42.053	-20.202	1.00	200.84
	2209	CD1	TRP A	87	-2.185 -2.292	41.854	-21.551	1.00	200.84
45	2210	NE1	TRP A	67 87	-3.942	40.645	-23.002	1.00	200.84
	2211	CZ2	TRP A	87	-5.726	39.602	-21.752	1.00	200.84 200.84
	2212	CZ3	TRP A	87	-5.095	39.899	-22.961	1.00	147.13
	2213	CH2	TRP A	87	-2.233	40.608	-16.017	1.00 1.00	147.13
-	2214	CO	TRP A	87	-1.040	40.785	-15.743	1.00	135.82
50		N	LEU A	88	-3.198	40.715	-15.108 -13.725	1.00	135.82
	2216 2217	CA	LEU A	. 88	-2.886	41.049	-13.366		139.19
	2218	CB	LEU A	88	-3,469	42.416 43.605	-14.1 11		139.19
	2219	CG	LEU A	88		43.803 44.912	-13.593		139.19
5:	5 2220	CD1	LEU .			43.608	-14.008	1.00	139.19
	2221	CD2	LEU A			39.996	-12.772		135.82
	2222	Ç	LEU A			39.439	-12.976		135.82 146.34
	2223	0	LEU A			39.710	-11.736		148.34
_	2224	N.	LEU A			38.737	-10.726	1.00	125.53
6		CA	LEU A			37.466	-10.820		125.53
	2226	CB CG	LEU A	-		36.431	-9.74		125.53
	2227	CD1	LEU A		9 -4.026	36.143	-9.71		125.53
	2228 2229	CD2	LEU A	-	9 -1.719	35.168	-10.00 -9.35		146.34
_	5 2230	C	LEU /	8 ۵		39.355	-9.33 -9.07		146.34
C	2230	ŏ	LEU /	A 8		39.903	-8.50		124.61
	2232	Ň	LEU A	д 9		39.282 39.862	-7.17	_	124.61
	2233	CA	LEU	A 9	0 -3.762		-6.68	1.90	89.03
	2234	СВ	LEU	A 9	0 -5.132 0 -5.136		-5.23		89.03
	70 2235	CG	LEU.	M 5	-5.130				

						-5.091	1.00	89.03
2000	CD1			, 104	41.932 41.132	-4.782	1.00	89.03
2236 2237	CD2). 	38.861	-6.196	1.00	124.61
2237	C			3.160	37.842	-5.902	1.00	124.61
2239	0			3.766 1.972	39.147	-5.686	1.00	143.99
5 2240	N	GG		1.335	38.229	-4.757	1.00	143.99
2241	CA		91	0.139	38.062	-5.110	1.00	163.37 163.37
2242	CB			0.382	37.527	-6.497	1.00 1.00	163.37
2243	CG	GLN A		1.861	37.383	-6.798 6.701	1.00	163.37
2244	CD OE1	GLN A	91	2.620	38.356	-6.721 -7.143	1.00	163.37
10 2245	NE2	GLN A		2.283	36.166	-3.304	1.00	143.99
2246 2247	C	GLN A	• •	-1.463	38.676 39.872	-2.991	1.00	143.99
2248	ŏ	GLN A		-1.322	37.706	-2.421	1.00	122.21
2249	N	ALA A		-1.725 -1.862	37.978	-0.991	1.00	122.21 218.43
15 2250	CA	ALA A		-3.283	37.702	-0.548	1.00	122.21
2251	СВ	ALA A ALA A	92	-0.892	37.128	-0.190	1.00 1.00	122.21
2252	C	ALA A	92	-0.653	35.960	-0.527 0.861	1.00	143.19
2253	O N	SER A	93	-0.338	37.733	1.742	1.00	143.19
2254	CA	SER A	93	0.612	37.067 37. 97 5	2.935	1.00	121.60
20 2255 2256 \	CB	SER A	93	0.964	37.975 38.446	3.608	1.00	121.60
2257	ŌĞ	SER A	93	-0.192	35.790	2.220	1.00	143.19
2258	C	SER A	93	-0.030 0.452	34.690	1.941	1.00	143.19
ي، 2259	0	SER A	93	-1.121	35.958	2.948	1.00	129.43 129.43
25 2260	N	ALA A	94 94	-1.880	34.831	3.446	1.00 1.00	204.58
2261	CA	ALA A ALA A	94	-1.688	34.686	4.950	1.00	129.43
2262	CB	ALA A	94	-3.322	35.190	3.108 2. 96 9	1.00	129.43
2263	C O	ALA A	94	-3.620	36.387	2.955	1.00	144.02
2264	N	GLU A	95	-4.208	34.193	2.632	1.00	144.02
30 2265 2266	CA	GLU A	95	-5.601	34.499 33.467	1.668	1.00	173.81
2267	СВ	GLU A	95	-6.144	33.492	0.344	1.00	173.81
2268	CG	GLU A	95 05	-5.434 -6.123	32.642	-0.695	1.00	173.81 173.81
2269	CD	GLU A	95 95	-5.590	32.539	-1.831	1,00	173.81
35 2270	OE1	GLU A	95	-7.201	32.078	-0.378	1.00 1.00	144.02
2271	OE2	GLU A	95	-6.488	34.587	3.879 3.857	1.00	144.02
2272	CO	GLU A	95	-7.548	35.222	4.963	1.00	165.64
2273 2274	Ň	VAL A	96	-6.044	33.951 33.966	6.222	1.00	165.64
40 2275	CA	VAL A	96	-6.778	32.573	6.592	1.00	130.98
2276	CB	VAL A	96	-7.256 -8.370	32.683	7.632	1.00	130.98 130.98
2277	CG1	VAL A	96 96	-7.722	31.830	5.359	1.00	165.64
2278	CG2	VAL A VAL A	96	-5.864	34.458	7.335	1.00 1.00	165.64
2279	C	VAL A	96	-4.743	33.962	7.475 8.147		117.82
45 2280	O N	VAL A	97	-6.339	35.404	9.204		117.82
2281 2282	CA	VAL A	97	-5.483	35.949 37.299	8.784	1.00	171.13
2283	СВ	VAL A	97	-4.908	37.597	9.605	1.00	171.13
2284	CG1	VAL A	97	-3.692 -4.577	37.296	7.307		171.13 117.82
50 2285	CG2	VAL A	97 97	-6.078	36.149	10.58		117.82
2286	C	VAL A VAL A	97	-7.269	36.404	10.71		130.77
2287	0	VAL A MET A		-5.221	36.046	11.60 13.02	_	130.77
2288	N CA	MET A		-5.592	36.228	13.92		249.69
2289	CB	MET A	98	-4.587	35.504 33.992	13.78		249.69
55 2290 2291	CG	MET A		-4.534	33.193	14.58		249.69
2292	SD	MET A	, 98	-5.915 -5.438	33.351	16.32		249.69 130.77
2293	CE	MET A	, 98 , 98	40	37.712	13.36		130.77
2294	Ç	MET A		4 500	38.332	13.10		130.20
60 2295	0	MET /			38.276	13.8		130.20
2296	N CA	GLU /	`	-6.679	39.701	14.19 15.1	4 00	216.65
2297	CB	GLU A	A 99	-7.773	39.989	15.1	• • • •	216.65
2298 2299	cG DO	GLU	A 99	- 444	41.423 41.757	16.3		216.65
65 2300	CD	GLU	A 99		40.074	16.7	95 1.00	216.65
2301	OE:		A 9		1	16.8		216.65 130.20
2302	OE:	2 GLU		9 -5.341	40.155	14.7		400.00
2303	C	GLU	• •	9 -4.832	39.538	15.6		4 = 0 00
2304		GLY	• • • •	00 -4.752		14.1	157 1.00	
70 2305	, 14	~- .		•				

				100	-3,476	41.685	14.674 13.8 6 9	1.00 1.00	150.30 150.30
	2306 2307	CA C	GLY A	100 100 100	-2.232 -1.210	41.342 42.016	13.999 13.043	1.00 1.00	150.30 149.89
	2308 2309	0 N	GLY A	101 101	-2.305 -1.173	40.305 39.891	12.209 11.699	1.00 1.00	149.89 220.06
5	2310 2311	CA CB	GLN A	101 101	-1.385 -1.255	38.471 37.429	12.777 13.650	1.00 1.00	220.06 220.06
	2312 2313	CD	GLN A GLN A	101 101	-0.056 -0.048	37.694 38.646	14.431 13.516	1.00 1.00	220.06 220.06
10	2314 2315	OE1 NE2	GLN A GLN A GLN A	101 101	0.974 -0.918	36.862 40.831	11.033 10.795	1.00 1.00	149.89 149.89
10	2316 2317	C O	GLN A PRO A	101 102	-1.663 0.161	41.773 40.572 39.692	10.277 10.571	1.00 1.00	131.84 202.39 131.84
	2318 2319	N CD	PRO A	102 102	1.289 0.440	41.436 41.376	9.131 9.067	1.00	202.39 202.39
15	2320 2321	CA CB	PRO A	102 102	1.966 2.222	39.941 40.960	9.395 7.837	1.00	131.84 131.84
	2322 2323	CG C	PRO A	102 102	-0.216 -0.418	39.749 41.915	7.627 6.960	1.00	120.38 120.38
20	2324 2325	0 N	LEU A	103 103	-0.531 -1.150	41.589 41.909	5.699 5.78	2 1.00	119.50 119.50
	2326 2327	CA CB CG	LEU A	103 103	-3.321	41.329 39.821	4.56 4.68	6 1.00	119.50
_	2328 2329	CD1 CD2	LEU A LEU A	103 103	4./53	41.816 42.345	4.47 4.50	8 1.00	120.38
25	2331	C	LEU A		3 -0.471	43.582 41.629	4.53 3.40	1.00	130.73
	2332 2333	N CA	PHE A	10	4 0.451	42.300 42.002	2.2 2.1 3.3	44 1.00) 196.69) 196.69
30	2334) 2335 2336	CB CG	PHE A	10	4 2.747	42.332 41.480	` 4.4	-	0 196.69 0 196.69
	2337 2338	CD1 CD2	PHE /	A 10	3.493	43.499 41.787	5.5	589 1.0 545 1.0	00 198.69
2	2339 5 2340	CE1 CE2	PHE PHE PHE	A 1	04 4.237 04 4.238		5.	638 1.0 004 1.0	00 130.73
3	2341 2342	CZ C		1	04 -0.236 04 -0.279	40.673	0		00 119.49
	2343 2344	0	LEU	A 1	05 -0.774 105 -1.42	42.514	-1	.066 1.	00 119.62
•	40 2345 2346	CA CB CG	LEU	A :	105 -2.813 105 -3.73	42.614	(172	.00 119.62 .00 119.62 .00 119.62
	2347 2348	CD1 CD2	LEU	Α	105 -5.13 105 -3.73 105 -0.57	8 41.092		2.137	.00 119.49 1.00 119.49
	45 2350	C	LEU LEU	A	105 0.09	1 44.10 14 42.44	\$ - 6 -	3.291	1.00 119.67 1.00 119.67
	2351 2352	N CA	ARC ARC	aΑ	106 -0.6 106 0.2 106 1.5	16 42.92 10 42.10	9 '	4.377	1.00 158.51 1.00 158.51
	2353 2354 50 2355	CB	AR	a A G A	106 2.5 106 3.6	13 42.48 56 41.50	3	-5.450	1.00 158.51 1.00 158.51
	50 2355 2356 2357	CD	AR AR	G A G A	106 4.5	322 41.79 231 40.8	76	-7.233 -6.860	1.00 158.51 1.00 158.51
	2358 2358	3 GZ	AF	IG A	106 5.	180 39.6 973 41.2	39	-8.280 -5.717	1.00 158.51 1.00 119.67 1.00 119.67
	55 236 236	O NF	AF	RG A RG A RG A	106 -0.	505 42.8 026 41.7	37	-6.069 -6.455	1.00 120.58
	236 236	2 O 3 N	C	YS A YS A	107 -1	.189 43.5	304	-7.774 -8.666	1.00 120.58
	60 236	ag C	C	YS A	107	.836 44.	299 304	-8.953 -8.168	1.00 140.98
	23 23	66 G	SB C	YS A	107	2.754 45.	384 210	-9.622 -9.083	1.00 148.29 1.00 148.29 1.00 148.29
	23	169	i l	HIS A	108	1 002 41	.644 .222	-9.914 -9.470	1.00 171.13 1.00 171.13
	2:	371	CB CG	HIS A	108	2.556 39 2.793 38	.660 3.483	-10.068 -10.691	1.00 171.13 1.00 171.13
	2	373	CD2 ND1	HIS A	108 108 108	3.773 40),308 9,549	-10.001 -10.548	1.00 171.13
		374 375	CE1	HIS A	,				

										171.13
			_		4.136	38.4		-10.975	1.00 1.00	148.29
	2376	NE2	HIS A	108 108	0.759	41.0		-11.411 -11.896	1.00	148.29
	2377	C O:	HIS A	108	-0.248	41.	229	-12.136	1.00	189.63 189.63
	2378 2379	N .	GLY A	109	1.701 1.593		286	-13.579	1.00 1.00	189.63
5	2378	CA	GLY A GLY A	109 109	2.109		002	-14.172 -13.469	1.00	189.63
,	2381	C	GLY A	109	2.735		,217 .782	-15.454	1.00	151.88
	2382	O N	TRP A	110	1.836 2.302		.582	-16.136	1.00	151.88 208.61
	2383 2384	CA	TRP A	110 110	1.381	39	.246	-17.307 -18.184	1.00 1.00	208.61
10	2385	СВ	TRP A	110	1.896		1.147	-18.170	1.00	208.61
	2386	CG CD2	TRP A	110	1.495		5.76 4 5.100	-19.135	1.00	208.61 208.61
	2387 2388	CE2	TRP A	110 110	2.277 0.556	36	5.022	-17.434	1.00 1.00	208.61
	2389	CE3	TRP A	110	2.863		3.255	-19.134 -19.708	1.00	208.61
15	2390	CD1 NE1	TRP A	110	3.103	_	7.034 4.723	-19.387	1.00	208.61 208.61
	2391 2392	CZ2	TRP A	110	2.147 0.429	3	4.653	-17.688	1.00 1.00	208.61
	2392	CZ3	TRP A	110 110	1.218	, 3	4.024	-18.658 -16.615	1.00	151.88
	2394	CH2	TRP A	110	3.747	, 3	19.773 10.909	-16.869	1.00	151.88 149.24
20	2395	C O	TRP A	110	4.182 4.490		38.666	-16.714	1.00 1.00	149.24
	2396 2397	N	ARG A	111	5.897	į ;	38.712	-17.125 -18.619	1.00	249.69
	2398	CA	ARG A	111	6.01	3	39.012	-19.494	1.00	249.69
	2399	CB CB	ARG A	111	6.01	4	37.777 38.106	-20.902	1.00	249.69 249.69
25	2400 2401	CD	ARG A	111		•	37.059	-21.427	1.00 1.00	249.69
	2402	NE	ARG A ARG A	111	- 40		36.693	-20.868 -19.757	1.00	249.69
	2403	CZ	ARG A	111	8.91		37.285 35.721	-21.411	1.00	249.69 149.24
0.0	2404	NH1 NH2	ARG A	111			39.777	-16.336	1.00 1.00	149.24
30) 2405 2406	C	ARG A	11 ¹			40.391	-16.825 -15.107	1.00	174.92
	2407	0	ARG A ASN A	11	2 6.2		39.988 40.958	-14.231	1.00	174.92 206.21
	2408	N CA	ASN A	11			40.434	-13.735		206.21
3	2409 5 2410	СВ	ASN A	11 11			41.184	-12.514 -12.171	4 00	206.21
٠,	2411	CG	asn a Asn a		2 8.2	201	42.258 40.620	-11.858	1.00	206.21
	2412	OD1 ND2	ASN A	. 1		703 029	42,283	-14.937		174.92 174.92
	2413 2414	Ċ	ASN A	•		992	43.001	-14.64° -15.86°		198.50
4	0 2415	0	ASN A	` .	13 6.	129	42.643	-15.60 -16.54	7 1.00	198.50
	2416	N CA	TRP	i 1	13 6.	.233 .232	43.932 44.051	-17.67	6 1.00	235.99 235.99
	2417 2418	CB	TRP			.232 .669	43.414	-18.92		235.99
	2419	CG	TRP		113 4	.825	42.775	-19.89 -20.96		235.99
	45 2420	CD2 CE2	TRP	Ä .	113 5	.653	42.372 42.498	-19.9	19 1.00	
	2421 2422	CE3	TRP	• •	,	3.455 3.927	43.381	-19.4	40 1.00 65 1.00	
	2423	CD1				6.931	42.753	-20.6 -22.0) 235.99
	2424	NE1 CZ2			113	5.150	41.705 41.837	-21.0	67 1.00	235.99
	50 2425 2426	CZ3	TRP	Α		2.952 3.801	41.452	-22.1	24 1.00 63 1.00	400 50
	2427	CH	TRP	A		5.948	45.050	-15.5 -14.3		198.50
	2428		TRP		113	5.891	44.821 46.262	-16.0	069 1.0	0 220.71
	2429 55 2430		ASP	Α	114	5.765 5.476	47.388	-15.		249.69
	55 2430 2431	CA		A	114 114	6.471	48.542	-15. -14	432 1.0 692 1.0	00 249.69
	2432	2 CB			114	7.802	48.353 48.237	-13.	446 1.0	00 249.69
	243		n ASF	A	114	7. 7 91 8.863	48.329	-15	.356	00 249.03
	243 60 243	`	D2 ASF	• A	114 114	4.037	47.881	40	.000	00 220.71
	243	6 C	4.01	? A ? A	114	3.569	48.065	4.4	242 1.	00 122.27
	243		1/4	LÂ	115	3.337	48.072 48.556	-14	1.268	440.42
	243 243	~ ~	A VA	L A	115	1.960 1.032	47.648	-13	,,,,,,	00 142.42
	65 24	က် င	a VA	L A L A	115 115	-0.418	47.95			00 142.42
	24	41		ĽΑ	115	1.328	46.195 49.97	. ·1	3.705 ¹	.00 122.27 00 122.27
	24 24	42 43	V/	T V	115 116	1.889 2.566	50.31	1 -1		1.00 122.27
	24	44) <u>V</u>	KL A	115 116	1.061	50.80	0 -1	4.336	
	70 24	4 5	4 17		•					

						52,181	-13.923	1.00	125.74 233.81
	0446	CA	TYR A	116	0.885 1.328	53.115	-15.058	1.00 1.00	233.81
	2446 2447	CD	TYR A	116 116	2.797	53.014	-15.357 -16.397	1.00	233.81
	2448	-	TYR A	116	3.272	52.218 52.092	-16.639	1.00	233.81
	2449	CD1	TYR A	116	4.644	52.092 53 683	-14.568	1.00	233.81 233.81
· 5	2450	CE1 CD2	TYR A	116	3.720 5.089	53.566	-14.796	1.00 1.00	233.81
	2451 2452	CE2	TYR A	116 116	5.551	52.773	-15.832 -16.054	1.00	233.81
	2453	CZ	TYR A TYR A	116	6.914	52.664 52.470	-13.539	1.00	125.74
_	2454	OH C	TYR A	116	-0.578	51.626	-13.747	1.00	125.74 145.27
10	2455	Ö	TYR A	116	-1.451 -0.833	53.665	-12.992	1.00 1.00	145.27
	2456 2457	N	LYS A	117 117	-2.176	54.095	-12.58·i -13.80 1	1.00	191.01
	2458	CA	LYS A	117	-3.020	54.515	-14.267	1.00	191.01
	2459	CB CG	LYS A	117	-2.807	55.955 56,437	-15.140	1.00	191.01 191.01
15	2460	CD	LYS A	117	-3.969 -5.304	56.363	-14.377	1.00 1.00	191.01
	2461 2462	CE	LYS A	117 117	-6.504	Ee 511	-15.161 -11.814	1.00	145.27
	2463	NZ	LYS A LYS A	117	-2.913	53.014	-12.141	1.00	145.27
	2464	CO	LYS A	117	-4.0 5 3	52.653 52.518	-10.767	1.00	149.03 149.03
20	2465	N	VAL A	118	-2.269 -2.858	51.469	-9.959	1.00 1.00	99.24
	2466 2467	CA	VAL A	118 118	-2.656 -1.761	50.002	-9.356 -8.081	1.00	99.24
	2468	CB	VAL A	118	-2.233	49.921	-10.374	1.00	99.24
	2469	CG1	VAL A	118	-1.364	49.558 51.912	-8.858	1.00	149.03 149.03
25	2470	CG2 C	VAL A	118		52.931	-8.179	1.00 1.00	111.25
	2471 2472	ŏ	VAL A	118 119		51.115	-8.706 -7.714	1.00	111.26
	2472	N	ILE A	119		51.325	-8.351	1.00	110.34
	2474	CA	ILE A	119	-7.15 7	51.950 52.293	-7.286	1.00	110.34 110.34
30	2475	CB CG2	ILE A	119		53.187	-9.108	1.00 1.00	110.34
	2476 2477	CG1	ILE A			53.537	-10.166 -7.162		111.26
	2478	CD1	ILE A		9 -6.349	49.972	-7.102 -7.919	1.00	111.26
	2479	C	ILE /	`	9 -6.641	49.054 49.843	-5.848	3 1.00	126.83 126.83
3:	5 2480	0 N	TYR /	12		48.603	-5.26		126.10
	2481 2482	ĞA		*	20 -6.829 20 -6.039	48.270	-4.01 -4.28		126.10
	2483	CB			20 -4.615	47.904	-4.39	9 1.00	126.10
	2484	CG		À 1	20 -3.636	48.884 48.542	-4.65	7 1.00	126.10 126.10
4	0 2485	CD1 CE1	TYR		20 -2.315 20 -4.243	46.569	-4.42		126.10
	2486 2487	CD2		• •	20 -4.243 20 -2.930	46.213	-4.68 -4.80		126.10
	2488	CE2			20 -1.968	47.197	-5.0	67 1.00	126.10
	2489	CZ	TYR	••	₁₂₀ -0.662		-4.8	B9 1.00	
4	45 2490	C OH	TYR	A	120 -8.280 120 -8.672	40.056	-4.6		
	2491 2492	ŏ	TYR		120 -8.6/2 121 -9. 08 4	47.753	-4.8 -4.5		106.78
	2493	N	TYR TYR	• •	121 -10.496	5 47.884	-5.7	734 1.00	155.39
	2494	CA CB	TYR	Â	121 -11.41		-6.7	1.00	
	50 2495	CG	TYP	l A	121 -11.36	1 49.122		459 1.00 499 1.00	455 20
	2496 2497	CD.		A	121 -10.18 121 -10.14	g 50.069	7	151 1.0	o 155.39
	2498			A	121 -12.51	6 49.522	-8.	187 1.0	0 155.39
	2499		5 TYI	A F	121 -12.49		. 45	858 1.0 903 1.0	
	55 2500 2501	, ~~	TY!	R A		F4 63	. 9	.903 1.0 .482 1.0	106.78
	2504	₂ O∺	1 1	R A	121 -11.2 121 -10.8	₉₂ 46.83	,	611 1.0	00 106.78
	2500	3 C		R A R A	121 -10.5	44 45.65	, A -2	.457 1.0	
	250		LY	SA	122 -11.6		2 •	1.410	00 141.82 00 249.31
	60 250 250	• •	A LY	'S A	122 -12.1 122 -11.5	11 46.67	4		00 249.31
	250 250	, c	B LY	is a Is a	122 -11.5	383 45.71		2.367 1	.00 249.31
	250	₂₈ C	~ .,	S A	122 -11.	631 46.2	20 20	3.451	.00 249.31 .00 249.31
	250	,,	E L	YS A	122 -12. 122 -12.	<i></i>	05	4.773	.00 249.31 .00 141.82
	65 25° 25		, L'	YS A	122 -12. 122 -13.	631 46.5	11	1.042	.00 141.82
	25 25	12 0	;	YS A YS A	122 -14	.136 47.5	· ·	-1.703	1.00 127.31
	25	13		SP A	123 -14	349 45.4	33	-1.701	1.00 127.31
			CA /	SP A	123 -15	i.801 ^{45.4}			
	70 25)13							

						400	C74	-0.276	1.00	199.26
		00	ASP A		-16.344		.574 .302	0.531	1.00	199.26
	516	CB CG	ASP A		-16.186		.223	0.031	1.00	199.26
	517	OD1	ASP A		-16.571		.378	1.668	1,00	199.26 127.31
	518 519	OD2	ASP A		-15.685 -16.395		3.531	-2.584	1.00	127.31
	2520	C	ASP A	123 123	-17,238	47	7.311	-2.132	1.00 1.00	152.83
	2521	0	ASP A GLY A	124	-15.955	: 46	3.579	-3.842 -4.788	1.00	152.83
	2522	N	GLY A	124	-16.468	3 47	7.561	-4.590	1.00	152.83
	2523	CA	GLY A	124	-16.06		9.007 9.847	-5.425	1.00	152.83
	2524	CO	GLY A	124	-16.39	•	9.047 9.297	-3.502	1.00	121.95
	2525	N	GLU A	125	-15.35	~ ~	0.668	-3.185	1.00	121.95 249.20
	2526 2527	ĊA	GLU A	125	-14.91 -15.03	-	0.926	-1.673	1.00 1.00	249.20
	2528	СВ	GLU A	125 125	-16.46	4 5	1.006	-1.143 -1.519	1.00	249.20
	2529	ÇG	GLU A	125	-17.15	;4	52.304	-1.081	1.00	249.20
15	2530	CD	GLU A	125	-16.68	,,,	53.373	-2.250	1.00	249.20
	2531	OE1 OE2	GLU A	125	-18.10	,,,	52.253 50.956	-3.612	1.00	121.95
	2532	C	GLU A	125	-13.4	, ,	50.071	-3.548	1.00	121.95 117.59
	2533 2534	ŏ	GLU A	125	-12.6 -13.2		52.185	-4.059	1.00	117.59
20	2535	Ň	ALA A	126 126	-11.8	~	52.572	4.444	1.00 1.00	242.07
20	2536	CA	ALA A	126	-11.9		53.935	-5.116	1.00	117.59
	2537	CB	ALA A ALA A	126	-11.1	02	52.638	-3.129 -2.132	1.00	117.59
	2538	C	ALA A ALA A	126	-11.6		53.123	-3.112	1.00	119.50
	2539	0 N	LEU A	127	-9.8		52.176 52.177	-1.857	1.00	119.50
25	2540	CA	LEU A	127			50.751	-1.411	1.00	117.16 117.16
	2541 2542	CB	LEU A	127		845 750	50.671	0.099	1.00	117.16
	2542	ČĠ	LEU A	127 127			51.245	0.705	1.00 1.00	117.16
	2544	CD1	LEU A	12	_	534	49.234	0.528 -1.813	1.00	119.50
30	2545	CD2	LEU A	12	_	859	52.960	-1,030	1.00	119.50
	2546	C	LEU A	12	7 -7.	.738	53.890 52.566	-2.616	1.00	140.05
	2547	0 N	LYS A	12		.880	53.269	-2.661	1.00	140.05 182.59
	2548 2549	CA	LYS A	12		.603 .503	52.411	-2.038		182.59
35	2549 2550	CB	LYS A	12		.725	52.060	-0.576		182.59
33	2551	CG	LYS A			1.526	53.260	0.337 1.80		182.59
	2552	CD	LYS A			4.657	52.855	2.74		182.59
	2553	CE	LYS A		28 ~	4.240	53.938 53.534	-4.12		140.05
	2554	NZ C	LYS A	\ 1		5.293	53.55 4 52.899	-5.01	0 1.00	140.05 141.11
40		ŏ	LYS /	•		5.875 4.386	54.467	-4.39		141.11
	2556 2557	Ň	TYR	•		4.021	54.780	-5.77		146.88
	2558	CA		•		4.977	55.812	-6.34 -7.57		146.88
	2559	CB				-4.437	56.491	-7.57 -8. 8 7		146.88
4:		CG			129	-4.560	55.909	-9.9		146.88
	2561	CD1 CE1	TYR	A		4.010	56.518 57.705	-7.4	74 1.00	
	2562	CD2	TYR	Α	129	-3.749	58.313	-8.5		
	2563 2564	CE2	TYR	A	129	-3.191 -3.327	57.717	-9.8	35 1.00 46 1.00	440.00
5	0 2565	CZ	TYR	À	129 129	-2.781	58.324	-10.9	10	
,	2566	ÓН	TYR TYR	A	129	-2.588	55.294	-5.9 -5.1		n 141.11
	2567	Č	TYR	Â	129	-2.098	56.070	·7.0		0 137.60
	2568	O N	TRP	Ä	130	-1.919	54.861 55.292		₂₈₂ 1.0	
	2569	CA	TRP	Α	130	-0.545 0.487	54.377		621 1.0	407.40
	55 2570 2571	CB	TRP	Ą	130	0.467	54.027	•	190 1.0 060 1.0	~
	2572		TRP		130 130	0.940	54.526		060 1.0 ,911 1.0	407.40
	2573	CD		A	130	0.426	53.878		.892 1.0	00 197.40
	2574	CE		Â	130	1.974	55.458		.702 1.	00 197.40
	60 2575		~	À	130	-0.661	53.124 53.018		.335 1.	00 197.40
	2576		·	> A	130	-0.561	54.128	-1	.624 1.	00 197.40 00 197.40
	2577		TRI	P A	130	0.893 2.452	55.713			
	2578 2579		73 TR	PA	130	1.906	55:055			.00 197.40 .00 137.60
	65 258	·	H2 TR	PA	130 130	-0.262	55.287		J.1	.00 137.60
	258	ı1 C		P A P A	130	-1.055	54.764			00 159.17
	258		-	RA	131	0.879	55.868 55.920		0.554 1	.00 159.17
	258			R A	131	1.313	400	' .	0.798	.00 169.09
	258 70 258	· · _		R A	1,31	2.164	37.10	•		
	70 258									

TEST.

2	586 587	CG CD1 CE1:	TYR A TYR A TYR A	131 131 131	2.407 1.394 1.603	57. 58.	426 927 .144 .150	-12.241 -13.051 -14.415 -12.821	1.00 1.00 1.00 1.00	169.09 169.09 169.09 169.09 169.09
5 2	2588 2589 2590 2591 2592	CD2 CE2 CZ OH	TYR A TYR A TYR A TYR A	131 131 131 131	3.642 3.863 2.842 3.073 2,152	57 57 58	.363 (.858 (.051 (.655	-14.183 -14.974 -16.318 -10.756	1.00 1.00 1.00 1.00 1.00	169.09 169.09 159.17 159.17
10	2592 2593 2594 2595 2596 2597	C O N CA CB	TYR A TYR A GLU A GLU A GLU A	131 131 132 132 132 132	1.619 3.464 4.328 5.777 6.593	55 55 55 7 55 7 5	3.613 4.754 3.577 3.933 4.598	-11.140 -10.524 -10.594 -10.237 -11.341 -11.767	1.00 1.00 1.00 1.00 1.00	172.97 172.97 249.69 249.69 249.69
15	2598 2599 2600 2601	CG CD OE1 OE2 C	GLU A GLU A GLU A GLU A	132 132 132 132	7.78- 8.09 8.41 3.67 3.53	4 5 7 5 1 5	3.750 2.767 54.063 52.838 53.413	-11.058 -12.804 -9.436 -8.343	1.00 1.00 1.00 1.00 1.00	249.69 249.69 172.97 172.97 204.08
20	2602 2603 2604 2605 2606	O N CA CB CG	GLU A ASN A ASN A ASN A	132 133 133 133 133	3.28 2.55 1.83 2.70	55 59 39 05	51.580 50.925 49.637 48.389 48.418	-9.628 -8.545 -9.065 -9.085 -9.493	1.00 1.00 1.00 1.00	204.08 217.94 217.94 217.94
25	2607 2608 2609 2610 2611	OD1 ND2 C O	ASN A ASN A ASN A ASN A HIS A	133 133 133 133 134	3.89 2.1 3.2 4.3 2.5	14 29 22	47.262 50.722 51.214 50.050	-8.676 -7.190 -6.922 -6.314 -4.979	1.00 1.00 1.00 1.00 1.00	217.94 204.08 204.08 188.50 188.50
30	2612 2613 2614 2615 2616	N CB CG CD2	HIS A HIS A HIS A HIS A	134 134 134 134	2.4 3.0 2.4	986 134 005 405 338	49.818 50.910 50.881 50.671 51.055	-4.067 -2.679 -1.481 -2.429 -1.120	1.00 1.00 1.00 1.00	249.69 249.69 249.69
35	2617 2618 2619 2620 2621	ND1 CE1 NE2 C O	HIS A HIS A HIS A HIS A	134 134 13 13	4 4. 4 3. 4 2. 4 2.	557 399 .485 .068 .518	50.953 50.720 48.456 47.636 48.217	-0.530 -4.542 -5.374 -3.234 -2.670	1.00 1.00 1.00 1.00	249.69 188.50 188.50 122.11 122.11
40	2622 2623 2624) 2625	N CA CB CG OD1	ASN A ASN A ASN A ASN A	13 13 13 13	35 2 35 3 35 3	2.076 3.274 3.803 3.010 5.128	46.946 45.986 45.530 45.158 45.534	-2.547 -3.90 -4.77 -4.08	7 1.0 6 1.0 6 1.0 6 1.0	0 249.69 0 249.69 0 249.69 0 249.69
4:	2626 2627 2628 2629 5 2630	ND2 C O N	ASN ILE	A 1 A 1 A 1	35 35 36 36	1.431 2.081 0.151 0.653	47.190 47.042 47.572 47.846 47.756	-1,30 -0,27 -1,31 -0,11 -0,48	1 1.0 3 1.9 5 1.5 52 1.0	00 122.11 00 110.87 00 110.87 00 153.19
	2631 2632 2633 2634 (0) 2635	CA CB CG2 CG1 CD1	ILE ILE ILE ILE	A 1 A A	136 136 136	-2.147 -2.474 -2.973 -4.463 -0.350	46.406 47.969 47.811 46.912	-1.0 0.8 0.5 1.0	55 1. 01 1. 53 1. 75 1	00 153.19 .00 153.19 .00 153.19 .00 110.87 .00 110.87
	2636 9537 2638 2639	C O N CA CB	ILE ILE SER SER SER	A A A	136 137 137 137	-0.773 0.351 0.763 2.242 2.597	45.732 47.475 46.734 46.951 46.432	2.0 3.2 3.4 4.7	254 1 488 1 746	1.00 139.22 1.00 139.22 1.00 151.42 1.00 151.42
	55 2640 2641 2642 2643 2644	0G C 0 N	SER SER ILE	Α	137 137 137 138 138	0.032 -0.378 -0.080 -0.760	47.027 48.149 45.991 46.072	4. 5. 6.	823 374	1.00 139.22 1.00 158.60 1.00 158.60 1.00 139.81
	60 2645 2846 2647 2644 264		1LE 32 ILE 31 ILE 01 ILE	A A A	138 138 138 138 138	-2.136 -2.695 -3.058 -4.349 0.014	45.423 45.183 46.314 45.652 45.396	7 5 5	.958 .766 .392 7.780	1.00 139.81 1.00 139.81 1.00 139.81 1.00 158.60 1.00 158.60
	65 265 265 265 265	0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ILE TH A TH B TH	R A R A IR A	138 139 139 139	0.321 0.309 1.053 1.698	44.203 46.174 45.695 46.87 47.85	7	3.816 9.975 0.697 0.990	1.00 172.47 1.00 172.47 1.00 249.69 1.00 249.69
	70 265	~ ~	G1 Th	IR A	139	0.689	,,,,,,,			

							9.811		249.69
			THR A	139	2.763	47.522 44.974	10.920	1.00	172.47
	2656	CG2 C	THR A	139	0.107	43.744	10.930	1.00	172.47 189.96
	2657	ο·.	THR A	139	0.027 -0.601	45.760	11.719	1.00 1.00	189.96
	2658 2659	N	ASN A	140 140	-1.573	45.233	12.662 13.830	1.00	189.00
5	2660	CA	ASN A	140	-1.738	46.209	14.835	1.00	189.00
3	2661	CB	ASN A	140	-2.767	45.750 45.403	14.466	1.00	189.00
	2662	CG OD1	ASN A	140	-3.887	45.764	16.111	1.00	189.00 189.96
	2663 2664	ND2	ASN A	140	-2.398 -2.877	45.113	11.879	1.00 1.00	189.96
10	2665	С	ASN A	140 140	-3.367	46.110	11.335 11.818	1.00	161.77
10	2666	0	ASN A ALA A	141	-3.437	43.904 43.674	11.062	1.00	161.77
	2667	N GA	ALA A	141	-4.669	42.364	10.287	1.00	147.99 161.77
	2668	CB	ALA A	141	-4.569 -5.962	43.694	11.874	1.00 1.00	161.77
15	2669 2670	č	ALA A	141 141	-6.105	42.992	12.888 11.402	1.00	148.72
13	2671	0	ALA A THR A	142	-6.902	44.510	12.032	1.00	148.72
	2672	N	THR A	142	-8.208	44.652 46.049	11.793	1.00	197.74 197.74
	2673	CA CB	THR A	142	-8.792 -7.820	47.046	12.140	1.00	197.74
20	2674 2675	OG1	THR A	142	-10.036	46.245	12.636	1.00 1.00	148.72
20	2675 2676	CG2	THR A	142 142	-9.126	43.636	11.376 10.277	1.00	148.72
	2677	C	A RHT	142	-8.849	43.153	12.037	1.00	167.20
•	2678	0	VAL A	143	-10.224	43.310 42.347	11.456	1.00	167.20
	2679	N CA	VAL A	140	-11.143	41.824	12.479	1.00	139.08 139.08
25	2680	CB	VAL A	143	-12.142 -13.146	42.910	12.826	1.00 1.00	139.08
	2681 2682	CG1	VAL A	143 143		40.590	11.934 10.334	1.00	167.20
	2683	CG2	VAL A VAL A	143		43.001	9.446	1.00	167.20
	2684	C	VAL A VAL A	143	-12.432	42.315 44.327	10.372	1.00	193 <i>.2</i> 7 193 <i>.2</i> 7
30	2685	0 N	GLU A	144		45.043	9.333	1.00	249.50
	2686	CA	GLU A	144		46.488	9.742	1.00 1.00	249.50
	2687 2688	CB	GLU A	144		46.624	11.002 12.141	4.00	249.50
	2689	CG	GLU A			47.202	12.003		249.50
3:		CD	GLU A	•	4 -12.590	48.352 46.511	13.170	1.00	249.50 193 <i>.2</i> 7
	2691	OE1 OE2	GLU /	ų 14		45.019	8.019		193.27
	2692	C	GLU A	A 14		45.370	6.98		179.52
	2693 2694	ŏ	GLU (A 14 A 14		44.606	8.06 6.86		179.52
Δ	μ) 2695	N	ASP ASP		9.931	44.524	7.22		162.18
7	2696	CA	ASP	•	45 -8.449		7.66	7 1.00	162.18 162.18
	2697	CB	ASP	A 1	45 -7.836	40.000	6.88		162.18
	2698	OD1	ASP	•	45 -7.903 45 -7.286	40 750	8.79	36 1.00 30 1.00	179.52
	2699 45 2700	OD2	ASP		45 -7.286 45 -10.357	43.348	6.00 4.8		179.52
	2701	C	ASP ASP		45 -10.00	3 43.286	6.5		145.41
	2702	.0	SER		46 -11.11		5.8	86 1.00	145.41 152.87
	2703	N CA	SER	Α ΄	146 -11.60 146 -12.31	•	6.8		152.87
	50 2705	CB	SER	• • •	146 -12.31 146 -11.47	7 39.816	7.9 4.7		145.41
	2706	OG	SER SER	• • •	146 -12.56	5 41.619		37 1.00	145.41
	2707		SEF		146 -13.51	8 42.349		563 1.00	168.10
	2708		GLY		147 -12.3	44 477	2.4	467 1.00	168.10 168.10
	2709 55 2710	^ ^	GLY	/ A	147 -13.2°		1.	149 1.00 129 1.60	400 10
	55 2710 2711	C	GL'	A	147 -12.0	11 39.807	^	129 1.00 048 1.00	117.05
	271	2 0	77.11	Y A R A	148 -13.3	06 41.425	'	2B3 1.00	117.05
	271			R A	148 -12.9		•	.014 1.00	
	271		a TH	R A	148 -14.2 148 -14.3	44 44	2	.867 1.00	446 30
	60 271 271	~	G1 TH	R A	148 -14.4 148 -15.5	40.05	9 -]	.012 1.00	117.05
	271	7 0	G2 TF	A AI	148 -123	235 42.00	7	2.116 1.0 2.502 1.0	0 117.05
	27	18		A AI	148 -12.	B33 43.01	٠ ,	2.386 1.0	0 131.53
	27	19	יר אינו ייר	/R A	149 -10.	40.7	5	3.128 1.0	404.04
	65 27	20	T T	YR A		136 42.73 .772 42.90	o6 -	2.453 1.0 1.003 1.0	104.84
	27		œ T	YR A		ens 43.3	38 -	1.003 1.0 0.010 1.0	00 104.84
		23	_	A RY	149 -9	.126 42.4	~	1.361	
	27	r24 '	CD1 T CE1 T	YR A YR A	149 -8	.127 42.8	د ی		
	70 27	725	J. '						

	2726	CD2	TYR A	149 149	-8.477 -8.467	44.6 45.0	42	-0.639 0.700 1.696	1.00 1.00 1.00	104.1 104.1 104.	84 84
	2727	CE2 CZ	TYR A	149	-8.792	44.1 44.5		3.019	1.00 1.00	104. 131.	
	2728 2729	OH	TYR A	149 149	-8.778 -9.881	42.3	37 i	-4.589 -4.989	1.00	131	.53
5	2730	CO	TYR A TYR A	149	-10.064	41.2 43.3		-5.362	1.00 1.00	105 105	.68 .68
	2731 2732	N	TYR A	150 150	-9.454 -9.0 9 0	43.	272	-6.784 -7.660	1.00	139	.51
	2733	CA	TYR A	150	-10.319		023 2 31	-7.964	1.00	139),51),51
10	2734	CB CB	TYR A	150 150	-11.173 -10.738	45.	.210	-8.856 -9.205	1.00 1.00	139	9.51
10	2735 2736	CD1	TYR A	150	-11.568		.306 .369	-7.413	1.00		9.51 9.51
	2737	CE1 CD2	TYR A	150	-12.456 -13.294	45	.456	-7.759 a 660	1.00 1.00	13	9.51
	2738 2739	CE2	TYR A	150 150	-12.839		3.418 7.460	·8.660 -9.041	1.00		9.51
15	2740	CZ OH	TYR A	150	-13.648 -8.429		7,469 4,587	-7.146	1.00 1.00		5.68 5.68
	2741 2742	C	TYR A	150 150	-8.720		5.604	-6.525 -8.128	1.00		9.57
	2743	0	TYR A	151	-7.536		4.585 5.830	-8.510	1.00 1.00		99.57 99.57
20	2744 2745	N CA	CYS A	151 151	-6.868 -6.994	4	6.133	-9.992 -10.786	1.00		99.57
20	2745 2746	С	CYS A	151	-7.274		5.244 15.773	-8.136	1.00		48.54 48.54
	2747	CB O	CYS A	151			14.452	-8.958 -10.359	1.00 1.00	1	07.45
	2748 2749	SG	CYS A THR A	151 152	-6.782		47.396 47.838	-11.756	1.00		07.45 135.55
25	2750	N CA	THR A	152	2 -6.857		47.650 48.753	-11.986	1.00 1.00		135.55 135.55
	2751 2752	CB	THR A	15	~ ~	2	50.045	-11.407 -11.345	1.00		135.55
	2753	OG1 CG2	THR A	15	2 -9.29	,	48.160 48.637	-12.118	1.00		107.45 107.45
2	2754 () 2755	C	THR A	15			49.358	-11.285 -13.359		,	123.72
3	2756	0	THR /	`	კ ვ -5.15		48.518 49.241	-13.744	1.00		123.72 123.72
	2757	N CA	GLY 4	A 1:	₅₃ -3.97 53 -3.74		49.248	-15.239 -15.96			123.72
	2758 2759	С	GLY GLY	n :	53 -4.38	38	48.477 50.113	-15.69	1 1.0	0	129.98 129.98
3	35 2760	0 N	LYS	A 1	54 -2.86 54 -2.5		50.256	-17.10 -17.48	7 1.0		212.29
	2761 2762	CA	LYS LYS		54 -2.4	90	51.740 52.012	-17.40	5 1.0	Ю	212.29 212.29
	2763	CB CG	LYS	Ä 1	154 -2.2		53.502	-19.22	25 1.0		212.29
	2764 40 2765	CD	LYS		154 -2.3 154 -2.0		53.803	-20.69 -20.99		00	212.29
	2766	CE NZ	LYS	Ä	154 -2.1		55.266 49.591	-17.4	45 1.	00 00	129.98 129.98
	2767 2768	C	LYS	,,	154 -1. 154 -0.	130	49.969	-18.9 -18.3		.00	168.08
	2769	0	LÝS VAL		155 -1.	242	48.579 47.827	-18.7	69 1	.00	168.08 187.90
	45 2770		VAL	. A		071 ,355	46.305	-18.7 -19.5		.00 .00	187.90
	2771 2772	CB			155 0	.825	45.540 45.849	-17.	343 1	.00	187.90 168.08
	277	3 66	VAL	_ A	100	.658 .193	48.277	-20. -21.		1.00	168.08
	50 277	c c	VAI VA		155 -0	.717	48.244 48.672	-21. -20.	493	1.00	179.87 179.87
	277	6 0	TR	PA	156	1.429 1.765	49.167	-21	.834	1.00 1.00	249.69
	271 271	'a C	A TR	PA		1.399	48.169		.954 .019	1.00	249.69
	27	79 CI	TF.	IPA RPA	156	2.200	46.890 46.752	-23	.359	1.00 1.00	249.69 249.69
	55 271 27	~	no TF	RP A		3.591 3.900	45.367	-23	3.302 3.714	1.00	249.69
	27	82 C		RPA RPA	156	4.606	47.657 45.625	-2	2.774	1.00	249.69 249.69
	27		ni T	RP A	156 156	1.740 2.754	44.707		2.945 3.581	1.00 1.00	249.69
		785 N	NE1 T	RP A RP A	156	5.175	44.871 47.161	-2	3.993	1.00	249.69 249.69
	2	786	C73 T	RP A	156	5.876 6.148	45.779	2	23.921	1.00 1.00	179.87
		788	CH2	RP A	156 156	0.905	50.400	,	22.020 21. 53 5	1.00	179.87 176.07
	2	789	Š	RP A	156	1.242	51.485 50.212	2	22.712	1.00 1.00	176.07
		2790 2791	Ň	GLN A	157 157	-1.161	51.30	1 .	22.959 24.313	1.00	249.69
	:	2792	CB	GLN A GLN A	157	-0.864	51.95 52.85		24.311	1.00 1.00	249.69 249.69
		2793 2794	CG	GLN A	157 157	0.381 0.232	54.07		-23.412	1.00	_,,,,,,
		27 95	CD	GLN A	101		•				

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	796	OE1 NE2	GLN A GLN A	157 157	-0.638 1.086	54.922 54.180 50.904	-23.635 -22.391 -22.872	1.00 1.00 1.00	249.69 249.69 176.07
	797 798	C	GLN A	157	-2.643 -3.504	51.584	-23.430	1.00	176.07 185.71
	799 2799	0	GLN A	157 158	-2.937	49.811	-22.171	1.00 1.00	165.71
	2800	N	LEU A	158	-4.320	49.375	-21.989 -22.809	1.00	232.32
	2801	CA CB	LEU A	158	4.51	48.122 48.278	-24.317	1.00	232.32
	2802	CG	LEU A	158	-4.80 9	47.274	-24.764	1.00	232.32
	2803 2804	CD1	LEU A	158	-5.868 5.267	49.687	-24.663	1.00	232.32 165.71
	280 5 2805	CD2	LEU A	158 158	-5.267 -4.642	49.105	-20.520	1.00	165.71
	2806	C	LEU A	158	-3.764	48.726	-19.741 -20.148	1.00 1.00	172.26
	2807	0	ASP A	159	-5.903	49.301	-18.772	1.00	172.26
	2808	N CA	ASP A	159	-6.321	49.080 49.974	-18.431	1.00	159.32
15	2809	CB	ASP A	159	-7.518 -7.259	51.435	-18.725	1.00	159.32 159.32
15	2810 2811	CG	ASP A	159	-7.25 5 -6.345	52.022	-18.103	1.00	159.32
	2812	OD1	ASP A	159 159	-7.974	51.995	-19.586	1.00 1.00	172.26
	2813	OD2	ASP A ASP A	159	-6.76-	47.618	-18.556 -19.479	1.00	172.26
	2814	C	ASP A	159	-7.192	46.960 47.113	-17.343	1.00	165.86
20	2815	N	TYR A	160	-6.468	45.741	-17.016	1.00	165.86
	2816 2817	CA	TYR A	160	-6.826 -5.667	44.810	-17.253	1.00	170.32 170.32
	2818	CB	TYR A	160 160	-5.121	44.887	-18.643	1.00 1.00	170.32
	2819	CG	TYR A TYR A	160	-4.101	45.789	-18.959 -20.241	1.00	170.32
25	2820	CD1	TYR A	160	-3.558	45.844	-19.645	1,00	170.32
	2821	CE1 CD2	TYR A	160	-5.600	44.042 44.088	-20.937	1.00	170.32
	2822 2823	CE2	TYR A	160	-5.072 4.046	44.988	-21.228	1.00	170.32 170.32
	2824	CZ	TYR A	160 160	-4.046 -3.493	45.018	-22.495	1.00 1.00	165.86
30	2825	ÓН	TYR A	160		45.590	-15.586 -14.675	1.00	165.86
•	2826	C	TYR A	160	-6.845	46.289 44.660	-15.410	1.00	140.66
	2827	0 N	GLU A	161		44,380	-14.119	1.00	140.66
	2828 2829	CA	GLU A	161		44.448	-14.272	1.00	201.20 201.20
35	2830	CB	GLU A	161 161		44.125	-13.044	1.00 1.00	201.20
55	2831	cG	GLU A	16		44.551	-13.222 -12.499	1.00	201.20
	2832	CD OE1	GLU A	16	1 -13.525	44.011 45.434	-14.076		201.20
	2833	OE2	GLU A	16		42.987	-13.688	1.00	140.66 140.66
40	2834 2835	č	GLU A	16		42.095	-14.523		133.72
40	2836	0	GLU A	16 16		42.815	-12.389	1.00	133.72
	2837	N	SER A	16	2 -7.628	41.552	-11.841 -10.672		153.53
	2838	CA CB	SER A	16	32 -6.687	41.835 42.515	-9.61		153.53
45	2839	OG	SER A		32 -7.366	40.686	-11.34	1 1.00	133.72 133.72
45	2840 2841	Č	SER A		62 -8.766 62 -9.852	41.187	-11.06		190.14
	2842	0	SER A GLU A		62 -9.852 63 -8.517	39.386	-11.22 -10.69		190.14
	2843	N	GLU A	ìi	63 -9.539	38.488	-10.03		249.69
_	2844	CA CB	GLU /	١ 1	63 -9.037	37.041 36.372	-12.07	79 1.00	249.69
50	0 2845 2846	CG	GLU /	١ ١	63 -8.981 63 -10.356	36.015	-12.61	1.00	249.69 249.69
	2847	CD	GLU A		63 -10.356 63 -11.096	35.284	-11.97		249.69
	2848	OE1	GLU GLU	•	63 -10.694	38.462	-13.73 -9.2		190.14
	2849	OE2	GLU		163 -9.764	38.962 39.462	-8.6		190.14
5	5 2850	CO	GLU	A	163 -8.835	38.833	-8.7	36 1.00	116.57 155.66
	2851 2852	Ň	PRO	, ,	164 -10.991 164 -12.208	00 042	-9.4		116.57
	2853	CD	PRO	• •	164 -12.208 164 -11.302	39,267	-7.3 -7.3		
	2854	CA	PRO PRO		164 -12.814	39,411	-7.3 -8.2		155.66
(60 2855	CB			164 -13.205			325 1.00	116.57
	2856	c C	PRO	A	164 -10.827	- AT AEE	-6.	578 1.00	
	2857 2858	ŏ	PRO	Α	164 -10.820 165 -10.44	00 725		150 1.00	454 40
	2859	N	LEU		165 -10.44 165 -9.94	9 37.832		122 1.00 030 1.00	116.01
	65 2860	CA			165 -8.41	37.955	_	,030 1.00 .995 1.00	116.01
	2861	~~	1		165 -7.71	6 37.061 4 35.693	_	,953 1.0	0 116.01
	2862 2863		1 LEU	Α	165 -8.41 165 -6.24		3	.335 1.0	
	2864	Ç	D2 LEU	Α .	165 -6.24 165 -10.57			739 1.0	0 131.40
	70 286	5 C	LEU						

			40.661	39.156			151.49
2866	0		165 -10.651 166 -10.996	36.932			136.62
2867	N	7011		36.988			136.62
2868	CA:	ASN A	166 -11.583	35.861			179.00
2869	CB .	ASN A	166 -12.582	36.278		1.00	179.00
5 2870	CG	ASN A	166 -13.998 166 -14.338	37.458		1.00	179.00
2871	OD1	ASN A	166 -14.338 166 -14.839	35.305		1.00	179.00
2872	ND2	ASN A	166 -10.535	36.890		1.00	136.62 136.62
2873	С	ASN A	166 -9.561	36.155		1.00	136.70
2874	0	ASN A	167 -10.741	37.619		1.00	136.70
10 2875	N	ILE A	167 -9.795	37.605	2.521	1.00 1.00	129.99
2876	CA	ILE A	167 -8.857	38.814	2.472 3.694	1.00	129.99
2877	CB	ILE A	167 -7.953	38.809	1.209	1.00	129.99
2876	CG2 CG1	ILE A	167 -8.012	38.756	1.059	1.00	129.99
2879	CD1	ILE A	167 -7.114	39.934	3.867	1.00	136.70
15 2880 2881	C .	ILE A	167 -10.496	37.621 38.494	4.126	1.00	136.70
2882	ŏ	ILE A	167 -11.317	36.685	4.738	1.00	125.45
2883	N	THR A	168 -10.148 168 -10.808	36.66	6.016	1.00	125.45
2884	CA	THR A		35.424	6.131	1.00	120.45
20 2885	CB	THR A	168 -11.677 168 -12.602	35.394	5.041	1.00	120.45 120.45
2886	OG1	THR A	168 -12.451	35.445	7.433	1.00	125.45
2887	CG2	THR A THR A	168 -9.910	36.749	7.232	1.00 1.00	125.45
2888	C	THR A	168 -8.989	35.928	7.431	1.00	104.30
2889	0	VAL A	169 -10.194	37.757	8.050 9.276	1.00	104.30
25 2890	N	VAL A	169 -9.444	37.979	9.422	1.00	108.18
2891	CA CB	VAL A	169 -9.061	39.471	10.864	1.00	108.18
2892	CG1	VAL A	169 -8.798	39.826	8.602	1.00	108.18
2893	CG2	VAL A	169 -7.798	39.750 37.534	10.433	1.00	104.30
2894 30 2895	č	VAL A	169 -10.333	38.182	10.729	1.00	104.30
2896	Ö	VAL A	169 -11.331	36.416	11.069	1.00	193.03
2897	N	ILE A	170 -9.972 170 -10.727	35.860	12.191	1.00	193.03
2898	CA	ILE A	170 -10.727 170 -10.701	34.321	12.132	1.00	177.52 177.52
2899	CB	ILE A	170 -11.108	33.853	10.743	1.00 1.00	177.52
35 2900	CG2	ILE A ILE A	170 -9.291	33.800	12.404	1.00	177.52
2901	CG1	ILE A	170 -9.174	32.283	12.422 13.513	1.00	193.03
2902	CD1	ILE A	170 -10.133	36.337	13.542	1.00	193.03
2903	. C	ILE A	170 -9.014	36.850	14.614	1.00	156.56
2904 40 2905	Ň	LYS A	171 -10.858	36.172 36.621	15.921	1.00	156.56
40 2905 2906	ČA	LYS A	171 -10.335	37.705	16.466	1.00	223.67
2907	CB	LYS A	171 -11.244	37.247	16.553	1.00	223.67
2908	CG	LYS A	171 -12.675 171 -13.639	38.405	16.449	1.00	223.67 223.67
2909	CD	LYS A	171 -13.639 171 -13.412	39.423	17.548	1.00	223.67
45 2910	CE	LYS A	171 -14.415	40.529	17.484	1.00 1.00	156.56
2911	NZ	LYS A LYS A	171 -10.169	35.507	16.984	1.00	156.56
2912	Ç	LYS A	171 -9.911	35.776	18.164 -12.704	1.00	229.93
2913	0	NAG A	221 13.115	30.531	-12.704	1.00	229.93
2914	C1 C2	NAG A	221 13.292	32.012	-13.150	1.00	229.93
50 2915	N2	NAG A	221 11.991	32.635 33.943	-12.957	1.00	229.93
2916 2917	C7	NAG A	221 11.855	34.685	-12.679	1.00	229.93
2918	07	NAG A	221 12.801	34.518	-13.100	1.00	229.93
2919	C8	NAG A	221 10.451 221 14.066	32.185	-14.322	1.00	229.93
55 2920	C3	NAG A	14.054	33.560	-14.516		229.93 229.93
2921	03	NAG A		31.386	-14.319		229.93
2922	C4	NAG /	1	31.411	-15.666		229.93
2923	04	NAG A	45 45	29.925	-13.874 -12.623		229.93
2924	C5 O5	NAG A	44 000	29.895	-13.656		229.93
60 2925	C6	NAG	a 221 16.390		-12.701		229.93
2926	06	NAG	A 221 17.244		-15.90		249.69
2927 2928	C1	NAG	A 222 17.240	464	-16.91		249.69
2929	C2	DAM		450	-16.37	4 1.00	249.69
65 2930	N2	NAG		24.400	-16.20	5 1.00	249.69
2931	C7	NAG			-16.48		249.69 249.69
2932	07	NAG	40 741		-15.63		249.69
2933	C8	NAG NAG		B 32.023	-18.23		249.69
2934	CS	NAG	47 60		-19.21	1, 1.00	_ ,0.00
70 2935	03	10.0					

						00 574	-18.752	1.00	249.69
	2026	C4	NAG A	222	16.979	30.571 30.501	-19.878	1.00	249.69
	2936 2937	04	NAG A	222	16.114	29.634	-17.646	1.00	249.69
	2938	C5 :	NAG A	222	16.463	29.769	-16.459	1.00	249.69
	2939	O5 ·	NAG A	222	17.286 16.462	28.165	-18.038	1.00	249.69
	2940	C6	NAG A	222 222	15.210	27.555	-17.749	1.00	249.69
	2941	O6	NAG A	242	-3.871	18.493	-8.371	1.00	249.50 249.50
	2942	C1	NAG A NAG A	242	-3.270	18.370	-9.775	1.00 1.00	249.50
	2943	C2	NAG A	242	-1.860	18.040	-9.718 -10.287	1.00	249.50
4.0	2944	N2 C7	NAG A	242	-1.426	16.919	-10.862	1.00	249.50
10	2945	07	NAG A	242	-2.178	16.128	-10.205	1.00	249.50
	2946 2947	C8	NAG A	242	0.063	16.621 19.691	-10.511	1.00	249.50
	2948	C3	NAG A	242	-3.480 -2.951	19.600	-11.829	1.00	249.50
	2949	O3	NAG A	242	-2.851 -4.979	20.019	-10.567	1.00	249.50 249.50
15	2950	C4	NAG A	242 242	-5.159	21.345	-11.115	1.00 1.00	249.50
	2951	04	NAG A NAG A	242	-5.622	19.952	-9.158	1.00	249.50
	2952	C5 O5	NAG A	242	-5.285	18.711	-8.481 -9.2 3 5	1.00	249.50
	2953	C6	NAG A	242	-7.140	20.004	-8.725	1.00	249.50
20	2954	06	NAG A	242	-7.650	21.225 21.444	-12.280	1.00	249.69
20	2955 2956	C1	NAG A	243	-5.905	22.875	-12.441	1.00	249.69
	2957	C2	NAG A	243	-6.423	23.262	-11.323	1.00	249.69
	2958	N2	NAG A	243	-7.258 -7.047	24.432	-10.724	1.00	249.69 249.69
	2959	C7	NAG A	243 243	-6.150	25.215	-11.062	1.00	249.69
25	2960	07	NAG A NAG A	243	-7.964	24.787	-9.565	1.00 1.00	249.69
	2961	C8	NAG A	243		22.971	-13.739 -13.913	1.00	249.69
	2962	C3 O3	NAG A	243	-7.711	24,291	-14.888	1.00	249.69
	2963	C4	NAG A	243		22.613 22.760	-16.068	1.00	249.69
30	2964 2965	04	NAG A	243		21.178	-14.681	1.00	249.69
30	2966	C 5	NAG A	243		21.113	-13.392	1.00	249.69
	2967	O 5	NAG A	243 243		20.769	-15.727	1.00	249.69 249.69
	2968	C6	NAG A	24		21.598	-15.679	1.00	249.69
	2969	06	nag a Man a	24		23.132	-17.256	1.00 1.00	249.69
35	2970	C1 C2	MAN A	24		22,291	-18.199 -17.842	1.00	249.69
	2971	02	MAN A	24		22.309 22.695	-19.610	1.00	249.69
	2972 2973	C3	MAN A	24		22.695	-20.538	1.00	249.69
	2974	03	MAN A	24		24.155	-19.854	1.00	249.69
40		C4	MAN A	24 24		24,497	-21.200	1.00	249.69 249.69
	2976	04	MAN A	24		24.996	-18.895	1.00	249.69
	2977	C5	MAN A MAN A	_	4 -6.748	24.610	-17.507		249.69
	2978	O5	MAN A		44 -6.499	26.518	-19.137 -18.519		249.69
46	2979	C6 O6	MAN A	. 24	44 -7.631	27.105	-1.207		249.69
45	2980 2981	C1	NAG A		50 17.983	21.117 22.142	-0.738	1.00	249.69
	2982	C2	NAG A		50 19.036 50 19.037	22.235	0.709	1.00	249.69
	2983	N2	NAG A	•	50 19.037 50 20.062	21.752	1.406		249.69 249.69
	2984	C7	NAG A		50 21.042	21.214	0.870		249.69
50		07	NAG A	•	50 19.990	21.883	2.92		249.69
	2986	C8 C3	NAG A	•	250 18.721	23.516	-1.35 -1.00		249.69
	2987	03	NAG A		250 19.736	24.449	-2.87		249.69
	2988 2989	C4	NAG		250 18.617	23.400 24.648	-3.41		249.69
5	5 2990	04	NAG		250 18.193	00.000	-3.26	1.00	249.69
J	2991	C5	NAG	• •	250 17.612 250 17.986	21.032	-2.63		249.69 249.69
	2992	O5	NAG	• •	250 17.526 250 17.526		-4.75		249.69
	2993	C6	NAG NAG		250 16.887	20.775	-5.02		249.69
	2994	06	NAG		274 0.355		15.77 16.69	4.00	249.69
•	50 2995	C1 C2	NAG		274 -0.462		17.4		249.69
	2996 2997	N2	NAG		274 0.423	40.040	17.9		249.69
	2998	C7	NAG		274 -0.025	4	17.7	99 1.00	249.69
	2999	07	NAG		274 -1.188 274 0.966		18.7		
	65 3000	C8	NAG		274 0.96 274 -1.27		17.6	- 4.66	
	3001	C3	NAG NAG		274 -2.13	0 13.222	18.4		
	3002				274 -2.11	7 11.387	16.8 17.7		
-	3003			A	274 -2.76		451		
	70 3004			A	274 -1.22	. 10.596	,5	· · · · · · · · · · · · · · · · · · ·	
	, 0 3000	,			•				

						11.505	15.017	1.00	249.69
	2006	O5	NAG A	_	-0.517	9.637	15.026	1.00	249.69
	3006 3007	C6	NAG A	274	-2.018 -1.206	9.058	14.010	1.00	249.69
	3008	O6	NAG A	274 335	5.793	44.302	-4.488	1.00	249.69
	3009	C1	NAG A	335	6.924	43.869	-3.512	1.00	249.69 249.69
5	3010	C2	NAG A NAG A	335	6.696	44.490	-2.220	1.00 1.00	249.69
	3011	N2	NAG A	335	6.442	43.744	-1.148 -1.175	1.00	249.69
	3012	C7 O7	NAG A	335	6.394	42.513	0.156	1.00	249.69
	3013	C8	NAG A	335	6.211	44.481 44.222	-3.983	1.00	249.69
10	3014 3015	ထိ	NAG A	335	8.352	43.421	-3.281	1.00	249.69
10	3015	03	NAG A	335	9.296 8.520	43.993	-5.483	1.00	249.69
	3017	C4	NAG A	335 335	9.821	44.401	-5.897	1.00	249.69 249.69
	3018	04	NAG A NAG A	335	7.450	44.802	-6.205	1.00 1.00	249.69
	3019	C5	NAG A	335	6.149	44.255	-5.895 -7.718	1.00	249.69
15	3020	O5 C6	NAG A	335	7.609	44.762	-8.267	1.00	249.69
	3021	06	NAG A	335	7.688	46.071 46.639	17.035	1.00	249.69
	3022 3023	C1	NAG A	340	-3.087	45,639	18.030	1.00	249.69
	3024	C2	NAG A	340	-3.935 -4.856	44.975	17.311	1.00	249.69
20	3025	N2	NAG A	340 340	-4.830 -4.995	43.695	17.659	1.00	249.69 249.69
20	3026	C7	NAG A	340	-4.379	43.170	18.595	1.00	249.69
	3027	07	nag a Nag a	340	-5.979	42.868	16.843 18.927	1.00 1.00	249.69
	3028	C8	NAG A	340	-4.707	46.820	19.924	1.00	249.69
05	3029	C3 O3	NAG A	340	-5.434	46.110	19.596	1.00	249.69
25	3030 3031	C4	NAG A	340	-3.738	47.802 48.790	20.299	1.00	249.69
	3032	04	NAG A	340	-4.485 -2.841	48.473	18.533	1.00	249.69
	3033	C5	NAG A	340 340	-2.166	47.471	17.739	1.00	249.69 249.69
	3034	O 5	NAG A	340	-1.761	49.371	19,114	1.00	249.69
30	3035	C6	NAG A NAG A	340	-0.846	49.785	18.103	1.00 1.00	221.62
	3036	O6	NAG A	366	-16.179	35.618	-1.670 -2.761	1.00	221.62
	3037	C1 C2	NAG A	366	-16.600	34.642	-3.871	1.00	221.62
	3038 3039	N2	NAG A	366	-15.672	34.736 33.944	-3.922	1.00	221.62
35	3040	C7	NAG A	366		33.096	-3.062	1.00	221.62
55	3041	07	NAG A	366 366		34.112	-5.114	1.00	221.62 221.62
	3042	C8	NAG A NAG A	366	4	34.981	-3.236	1.00 1.00	221.62
	3043	C3	NAG A	366		33.973	-4.125 -2.065	1.00	221.62
	3044	03 C4	NAG A	366	-18.991	35.113	-2.557	1.00	221.62
40		04	NAG A	366		35.683 36.017	-0.964		221.62
	3046 3047	· C5	NAG A	360		35.560	-0.585	1.00	221.62
	3048	05	NAG A	36		36.056	0.304		221.62
	3049	C6	NAG A	36 36		37.042	1.205		221.62 249.69
4:	3050	06	NAG A NAG A	36		34.987	-2.286		249.69
	3051	C1	NAG A	36		35.932	-2.385 -1.478		249.69
	3052	C2 N2	NAG A	36	7 -22.437	37.053	-1.969	-	249.69
	3053 3054	C7	NAG A	. 36		38.275 38.512	-3.18	1 1.00	249.69
5	() 3055	. 07	NAG A	36		39.407	-0.96	6 1.00	249.69
,	3056	C8	NAG A	36	57 -23.858	35,142	-2.05		249.69 249.69
	3057	C3	NAG A	•	67 -24.998	35.986	-2.16		249.69
	3058	03	NAG A		67 -23.984	33.958	-3.03 -2.66		249.69
	3059	C4 O4	NAG A	•	67 -25.101	33.153	-3.01		249.69
3	3060 3061	C5	NAG A	A 3	67 -22.694	33.108 33.938	-3.25		249.69
	3062	O5	NAG /		67 -21.528	32.031	-4.00		249.69
	3063	C6	NAG A	-	167 -22.696 167 -21.707	32.291	-5.07		249.69 249.69
	3064	O6	NAG		367 -21.707 31.112	63.164	23.8		249.69
	60 3065	СВ	LYS	_	31.172	64.583	23.2		249.69
	3066	CG		_	4 31.232	65.658	24.3		249.69
	3067	CD	LYS	_	4 31.339	67.065	23.7 24.7		249.69
	3068	NZ.	LYS		4 31.384		21.9		249.69
	3069 65 3070	_	LYS	В	4 32.410		22.3	371 1.00	249.69
	3070 3071	_	LYS	В	4 33.409 4 31.072		23.4	434 1.00	
	3072	, N	LYS	В	4 31.072		22.7		
	3073	S CA	LYS PRO	B	5 32.38	61.656		698 1.00 128 1.00	
	3074			В	5 31.37		20.	128 1.00	, ,,,,,,,,
	70 3075	, 00			•				

				_ •	-0.500	61.750	19.825	1.00	223.70
3	076	CA		5	33.562 33.387	60.550	18.906	1.00	195.58
	1077	CB.		5	31.904	60.498	18.724	1.00	195.56
	078	CG.		5 5	33.598	63.077	19.060	1.00	223.70 223.70
3	3079	C	PRO B	5	32.576	63.741	18.895	1.00	208.07
	3080	0	LYS B	6	34.780	63.472	18.605 17.858	1.00 1.00	208.07
	3081	N CA	LYS B	6	34.916	64.713	18.783	1.00	245.96
	3082	CB	LYS B	6	35.357	65.849	18.074	1.00	245.96
	3083 3084	ca	LYS B	6	35.467	67.195 68.337	19.039	1.00	245.96
	3085	CD	LYS B	6	35.756	69.677	18.304	1.00	245.96
10	3086	CE	LYS B	6	35.816 35.973	70.834	19.231	1.00	245.96
	3087	NZ	LYS B	6 6	35.920	64.543	16.721	1.00	208.07 208.07
	3088	C	LYS B Lys b	6	37.122	64.371	16.946	1.00 1.00	211.91
	3089	0 N	VAL B	7	35.414	64,603	15.497 14.312	1.00	211.91
15	3090	CA	VAL B	7	36.245	64.443	13.053	1.00	105.28
	3091 3092	CB	VAL B	7	35.379	64.356 63.818	11.881	1.00	105.28
	3093	CG1	VAL B	7	36.218	63.495	13.325	1.00	105.28
	3094	CG2	VAL B	7 7	34.151 37.258	65.565	14.107	1.00	211.91
20	3095	C	VAL B VAL B	7	36.903	66.741	14.033	1.00	211.91 208.76
	3096	0	VAL B SER B	8	38.524	65.185	14.009	1.00 1.00	208.76
	3097	N CA	SER B	8	39.599	66.141	13.797 14.770	1.00	216.01
	3098	CB	SER B	8	40.749	65.846	14.777	1.00	216.01
25	3099 3100	OG	SER B	8	41.085	64.465 66.033	12.348	1.00	208.76
23	3100	C	SER B	8	40.084	65.031	11.685	1.00	208.76
	3102	Ō	SER B	8	39.830	67.061	11.853	1.00	194.89
	3103	N	LEU B	9	40.767 41.278	67.030	10.487	1.00	194.89 159.88
	3104	CA	LEU B	9 9	40.528	68.017	9.599	1.00 1.00	159.88
30	3105	CB	LEU B	9	39.017	67.914	9,401 8,190	1.00	159.88
	3106	CG CD1	LEU B	9	38.658	68.762	9.175		159.88
	3107	CD2	LEU B	9	38.575	66.489 67.363	10.413		194.89
	3108 3109	C	LEU B	9	42.760	67.981	11.315	1.00	194.89
35	3110	0	LEU B	9	43.318 43.390	66.956	9.319		186.22
55	3111	N	ASN B ASN B	10 10		67.229	9.113		186.22 231.85
	3112	CA	ASN B ASN B	10		66.253	9.914		231.85
	3113	CB CG	ASN B	10		66.704	10.01! 10.59		231.85
40	3114	OD1	ASN B	10		67.753 65.921	9.44		231.85
40	3115 3116	ND2	ASN B	10		67.123	7.63		186.22
	3117	С	ASN B	10		66.030	7.05		186.22
	3118	0	ASN B	10			6.99		188.99 219.87
	3119	N	PRO B	- 1		68.247	5.57		188.99
45	3120	CD CA	PRO B	1	1 45.592		7.53 6.28		219.87
	3121 3122	CB	PRO B	1			5.43		219.87
	3123	ČĞ	PRO B	1			8.20		188.99
	3124	C	PRO B	1			8.10	38 1.00	188.99
50	3125	0	PRO B		1 43.28 2 44.44		9.0		172.73 135.97
-	3126	N	PRO B		2 45.66	1 71.989	9.3		172.73
	3127	CD	PRO B		2 43.29	0 71.755	9.7		135.97
	3128	CA CB	PRO B		12 43.92		10.6 10.7		135.97
55	3129 5 3130	ČĠ	PRO B	•	12 45.37				172.73
3.	3131	Č	PRO B		12 42.27			17 1.00	172.73
	3132	0	PRO B		12 41.07 13 42.78		7.5	93 1.00	154.67
	3133	N	TRP B	}	13 42.70 13 42.00		6.5	503 1.00	154.67 165.26
	3134	CA	TRP E		13 42.9		5.3	300 1.00	165.26
6	0 3135	CB	TRP		13 44.2	49 74.215	,	858 1.00 873 1.00	165.26
	3136	CG CD2		3	13 44.4	55 75.194	•	650 1.00	165.26
	3137	CE2		3	13 45.8		´ -	601 1.00	165.26
	3138 3139	CE3	TRP	В	13 43.6		, _	073 1.00	165.26
6	5 3140	CD1	TRP		13 45.4		_	668 1.00	
·	3141	NE1	TRP	В	13 46.4 13 46.3	45	6 7.	.521 1.00	
	3142	CZ2		ម B	13 46.3 13 44.1		ვ 8	464 1.00	400.00
	3143	CZ3 CH2		В	13 45.5	506 77.08		.420 1.00 .088 1.00	
_	3144	CH2	TRP	B	13 40.1		10 B	.000 1.00	
	70 3145	J			•				

						•		5.593 °	1.00	154.67
		•	TRP B	13	41.023	71.414				126.91
	146	O N	ASN B	14	39.627	73.038 72.290			1.00	126.91
	147	CA:	ASN B	14	38.416	72.308			1.00	191.01
	148 149	CB	ASN B	14	37.397 36.877	73.687			1.00	191.01 191.01
	150	CG	ASN B	14 14	37.643	74.604			1.00 1.00	191.01
	151	OD1	ASN B ASN B	14	35.564	73.848		7.246 4.590	1.00	126.91
	1152	ND2	ASN B	14	37.778	72.796		4.336	1.00	126.91
	3153	C	ASN B	14	36.595	72.577 73.477		3.799	1.00	109.47
	3154 3155	Ň	ARG B	15	38.606 38.240	74.033		2.509	1.00	109.47 119.97
10	3156	CA	ARG B	15 15	38.096	75.576		2.571	1.00 1.00	119.97
	3157	CB	ARG B	15	37.202	76.153		3.671 3.482	1.00	119.97
	3158	CG	ARG B	15	37.010	77.677		2.444	1.00	119.97
	3159	CD NE	ARG B	15	36.034	78.008 79.040		1.615	1.00	119.97
15	3160 3161	CZ	ARG B	15	36.135 37.176	79.846		1.693	1.00	119.97 119.97
	3162	NH1	ARG B	15 15	37.176	79.273		0.715	1.00	109.47
	3163	NH2	ARG B	15	39.432	73.688		1.616	1.00 1.00	109.47
	3164	C	ARG B	15	40.462	74.353		1.689 0.769	1.00	122.07
20	3165	O N	ILE B	16	39.307	72.675 72.2 94		-0.072	1.00	122.07
	3166	CA	ILE B	16	40.431			0.303	1.00	121.17
•	3167 3168	CB	ILE B	16	40.914 41.691	TO 054		1.608	1.00	121.17 121.17
	3169	CG2	ILE B	16 16	39.708	69.975		0.377	1.00 1.00	121.17
25	3170	CG1	ILE B	16	40.058	68.526		0.495 -1.571	1.00	122.07
	3171	CD1	ILE B	16	40.20			-2.041	1.00	122.07
	3172	CO	ILE B	16	39.08			-2.314	1.00	169.19
	3173 3174	Ň	PHE B	17				-3.770	1.00	169.19 156.59
30	3175	CA	PHE B	17 17		72.815		-4.351	1.00 1.00	156.59
50	3176	СВ	PHE B PHE B	17		5 74.285		-4.609 -4.420	1.00	156.59
	3177	CG CD1	PHE B	17	43.88			-5.076	1.00	156.59
	3178	CD2	PHE B	17				-4.690	1.00	156.59
35	3179 3160	CE1	PHE B	17		-0.050		-5.349	1.00	156.59 156.59
22	3181	CE2	PHE B	17		36 77.013	3	-5.156	1.00 1.00	169.19
	3182	CZ	PHE B	1		70. 94 7	<u>'</u>	-4.258 -3.460	1.00	169.19
	3183	CO	PHE B	1	7 40.8			-5.575	1.00	133.30
40	3184 3185	N	LYS B	1		50 50		-6.208	1.00	133.30
40	3186	CA	LYS B		8 40.5 8 39.9	• • • • • • • • • • • • • • • • • • • •	7	·7.575	1.00	237.07 237.07
	3187	CB	LYS B		8 39.9 8 39.5	00 68.53		-8.339	1.00 1.00	237.07
	3188	CG	LYS B		8 38.7	₂₀ 68.92		-9.585 -10.424	1.00	237.07
	3189	CE	LYS B		18 38.3			-11.054	1.00	237.07
45	3190 3191	NZ	LYS B		18 39.1 18 41.1			-6.363	1.00	133.30 133.30
	3192	C	LYS E	-	18 41.1 18 42.1	44		-6.884	1.00	182.54
	3193	0	LYS E			799 67.44		-5.899 -6.017		182.54
	3194	N CA	GLY E		19 42.	942 66.5		-0.017 -4.794		182.54
50	3195	C	GLY (3		823 66.4 703 65.6	80 42	-4.724	1.00	182.54
	3196 3197	ŏ	GLY 1	В		.703 65.6 .591 67.3		-3.835	1.00	116.49 116.49
	3198	N	GLU GLU	B 0		.396 67.4	24	-2.600		185.38
	3199	CA	GLU	B B		.276 68.8		-1.920 -2.82		185.38
5	5 3200	CB CG	GLU	В		.484 70.0		-2.04		185.38
	3201 3202	ÇD	GLU	В				-1.28	8 1.00	185.38 185.38
	3203	OE1				3.513 /1.3 5.433 72.	125	-2.20		116.49
	3204	OE2	GLU GLU	B B		3.948 66.	330	-1.62		116.49
6	0 3205	C	GLU	В		2.816 65.	854	-1.72 -0.66		130.57
	3206	0	ASN		21 4	7.010	.944 .911	0.30		130.57
	3207 3208	CA	ASN	В			.791	0.3	53 1.00	248.12 248.12
	3209	CB		В		3.7/0	.492	-0.9		240.40
	65 3210	CG	4041			5.414 63	.347	-2.0 -0.9		240 40
	3211			В	21 4	7.420 63	.384	-0.9 1.7		130.57
	3212		ASN	В	21 4	T-1-1-1-1-1	3.432 3.308	2.1	94 1.00	130.57
	3213 3214	·	ASN	I B			1.865		28 1.00	161.15
	70 321	* A1	VAL	. в	~~	T				

					42.933	65.242	3.810	1.00	161.15
;	3216	CA		22 22	42.833	66.157	3.876	1.00	160.53
;	3217	CB		22 22	40.447	65.365	3.549	1.00	160.53 160.53
	3218	CG1. CG2		22	41.584	66.778	5.249 4.652	1.00 1.00	161.15
_	3219	C	VAL B	22	42.633	64.002 63.035	4.052	1.00	161.15
5	3220 3221	ŏ	VAL B	22	42.062	64.041	5.940	1.00	186.22
	3222	N	THR B	23	42.985 42.771	62.898	6.849	1.00	186.22
	3223	CA	THR B	23 23	44.108	62.440	7.478	1.00	249.25
	3224	CB	THR B THR B	23	45.086	62.250	6.448	1.00	249.25 249.25
10	3225	OG1 CG2	THR B	23	43.919	61.136	8.238 8.004	1.00 1.00	186.22
	3226	C	THR B	23	41.804	63.173	8.783	1.00	186.22
	3227 3228	ŏ	THR B	23	42.015	64.109 62.345	8.132	1.00	183.26
	3229	Ň	LEU B	24	40.764	62.522	9.208	1.00	183.26
15	3230	CA	LEU B	24	39.782 38.339	62,398	8.677	1.00	177.01
	3231	CB	LEU B LEU B	24 24	37.949	62.842	7.258	1.00	177.01 177.01
	3232	CG	LEU B	24	36.435	62.918	7.183	1.00 1.00	177.01
	3233	CD1 CD2	LEU B	24	38.553	(190	6.910 10.329	1.00	183.26
20	3234 3235	C	LEU B	24	39.974	61.501 60.321	10.162	1.00	183.26
20	3236	ŏ	LEU B	24	39.661	61.965	11.472	1.00	238.46
	3237	N	THR B	25	40.476 40.717	61.111	12.636	1.00	238.46
	3238	CA	THR B	25 25	42.027	61.517	13.351	1.00	207.80
	3239	CB	THR B THR B	25	43.116	61.448	12.424	1.00	207.80 207.80
25	3240	OG1 CG2	THR B	25	42.312	60.594	14.527	1.00 1.00	238.46
	3241	C	THR B	25	39.562	61.234	13.632 13.949	1.00	238.46
	3242 3243	ŏ	THR B	25	39.133	62.342 60.099	14,126	1.00	203.48
	3244	N	CYS B	26	39.069 37.965	60.098	15.088	1.00	203.48
30	3245	CA	CYS B	26	37.965	60.356	16.500	1.00	203.48
-	3246	C	CYS B	26 26	39.563	59.880	16.861	1.00	203.48 181.40
	3247	0	CYS B	26	37.227	58.767	15.036	1.00 1.00	181.40
	3248	CB SG	CYS B	26	35.662	58.718	15.964 17.294	1.00	249.69
35	3249 3250	N	ASN B	27	37.708	61.100 61.472	18.666	1.00	249.69
33	3251	CA	ASN B	27	38.087	61.388	19.608	1.00	249.69
	3252	CB	ASN B	27	36.876 37.148	62.023	20.969	1.00	249.69
	3253	CG	ASN B	27 27	37.644	63.155	21.060	1.00	249.69 249.69
	3254	OD1	ASN B	27	36.820	61.299	22.033	1.00 1.00	249.69
40	3255	ND2 C	ASN B	27	39,259	60.677	19.254 19.837	1.00	249.69
	3256 3257	ŏ	ASN B	27	39.081	59.605	19.090	1.00	244.48
	3258	Ň	GLY B	28		61.234 60.619	19.577	1.00	244.48
	3259	CA	GLY B	28		61.439	19.026	1.00	244.48
45	3260	č	GLY B	28 28		61.561	17,809	1.00	244.48 249.69
	3261	0	ASN B	29		62.008	19.912		249.69
	3262	N CA	ASN B	29		62.853	19.497 20.698		249.69
	3263 3264	CB	ASN B	29		63.688 64.797	20.295		249.69
50		CG	ASN B	29		65.073	19.106	1.00	249.69
-	3266	OD1	ASN B	25		65.444	21.293		249.69
	3267	ND2	ASN B	2	45 020	62.076	18.865	1.00	249.69 249.69
	3268	C	asn b Asn b			62.412	17.75		249.69
5	3269 5 3270	N	ASN B	3	0 46.412	61.034	19.54 19.01		249.69
٥.	3270	ČA	ASN B	. 3	0 47.543	60.279 60.555	19.88		249.69
	3272	CB	ASN B	3	0 48.783 0 49.224	62.017	19.83	1 1.00	249.69
	3273	CG	ASN B		30 49.224 30 49.500		20.86		249.69 249.69
_	3274	OD1	ASN B ASN B		30 49.301	62.574	18.62		249.69
6	0 3275	ND2	ASN E	-	30 47.341	58.772	18.86		249.69
	3276	CO	ASN E		30 47.289		17.73 19.98		249.69
	3277 3278	Ň	PHE 6	3	31 47.227		19.93		249.69
	3279	CA	PHE	3	31 47.068		20.70		249.69
6	55 3280	CB	PHE		31 48.220 31 49.601		20.2	39 1.00	249.69
	3281	CG	PHE PHE		31 49.601 31 50.151	57.556	20.6		249.69 249.69
	3282	CD1 CD2			31 50.335	₅ 55.552	19.3		
	3283	CE1		B	31 51.400	3 57.9/6	20.2 18.8		
	3284 70 3285	CE2			31 51.589	9 . 55.967	10.0		
	, , , ,								

			DUE B	31 -	52,121	57.182	19.313	1.00	249.69 249.69
	3286	CZ.		31	45.718	56.071	20.433	1.00	249.69
	3287	Ç .		31	45.325	56.313	21.577	1.00	249.69
	3288	Ο.	PHE B PHE B	32	45.027	55.341	19.556	1.00 1.00	249.69
_	3289	N CA	PHE B	32	43.717	54.761	19.859 18.875	1.00	249.69
5	3290	CB	PHE B	32	42.670	55.314	19.304	1.00	249.69
	3291	CG	PHE B	32	41.238	55.081	20.443	1.00	249.69
	3292	CD1	PHE B	32	40.722	55.709	18.565	1.00	249.69
	3293 3294	CD2	PHE B	32	40.404	54.237 55.499	20.835	1.00	249.69
10	3295	CE1	PHE B	32	39.398	54.022	18.950	1.00	249.69
10	3296	CE2	PHE B	32	39.081 38.578	54.655	20.087	1.00	249.69
	3297	CZ	PHE B	32	43.771	53.220	19.785	1.00	249.69
	3298	C .	PHE B	32 32	44.746	52.646	19.285	1.00	249.69
	3299	0	PHE B	33	42.714	52.559	20.259	1.00	249.69 249.69
15	3300	N.	GLU B	33	42.688	51.104	20.273	1.00 1.00	249.69
	3301	CA	GLU B	33	42.563	50.633	21.724	1.00	249.69
	3302	CB	GLU B	33	42.965	49.185	21.932 21.285	1.00	249.69
	3303	CG CD	GLU B	33	44.299	48.858	21.471	1.00	249.69
20	3304	OE1	GLU B	33	45.257	49.641	20,593	1.00	249.69
20	3305 3306	OE2	GLU B	33	44.389	47.819 50.384	19.409	1.00	249.69
	3307	c_	GLU B	33	41.644	49.478	18.645	1.00	249.69
	3308	Ō	GLU B	33	41.991	50.773	19.532	1.00	249.69
	3309	N	VAL B	34	40.375 39.290	50.129	18.784	1.00	249.69
25	3310	CA	VAL B	34	37.920	50.767	19.158	1.00	247.84
	3311	CB	VAL B	34 34	36.794	50.060	18.427	1.00	247.84 247.84
	3312	CG1	VAL B	34	37.698	50.681	20.661	1.00	249.69
	3313	CG2	VAL B VAL B	34	39.448	50.119	17.252	1.00 1.00	249.69
	3314	C	VAL B	34	40.059	51.023	16.663	1.00	249.69
30	3315	0 N	SER B	35	38.895	49.077	16.627 15.175	1.00	249.69
	3316	CA	SER B	35	38.934	48.909	14.806	1.00	240.73
	3317	CB	SER B	35	39.389	47.500 46.555	15.104	1.00	240.73
	3318 3319	ŏĞ	SER B	35	38.373	46.555 49.126	14.625	1.00	249.69
35	3320	C	SER B	35	37.529	49.055	13.412	1.00	249.69
55	3321	0	SER B	35	37.305 36.583	49.371	15.533	1.00	249.69
	3322	N	SER B	36 36	35.186	49.611	15.162	1.00	249.69 249.69
	3323	CA	SER B SER B	36	34.233	48.825	16.081	1.00	249.69
	3324	CB	SER B SER B	36	34.184	49.372	17.391	1.00 1.00	249.69
40	3325	OG	SER B	36	34.857	51.108	15.231 16.278	1.00	249.69
	3326	C	SER B	36	34.462	51.639	14.102	1.00	249.69
	3327	Ň	THR B	37	35.037	51.780	14.004	1.00	249.69
	3328 3329	ČA	THR B	37	34.765	53.198 53.989	13.773	1.00	184.28
45	3330	CB	THA B	37	36.076	53.759	14.866	1.00	184.28
т.	3331	OG1	THR B	37		55.477	13.679		184.28
	3332	CG2	THR B	37 37		53.375	12.823		249.69
	3333	C	THR B	37		52.726	11.782		249.69 236.74
	3334	0	THR B	38		54.236	12.988		236.74
5	0 3335	N	LYS B	38		54.464	11.930 12.519		245.72
	3336	CA CB	LYS B	38	3 30.421	54.378	13.196		245.72
	3337	CG	LYS B	38	30.118	53.037	13.84		245.72
	3338 3339	čõ	LYS B			52.984 51.615	14.41		245.72
5	5 3340	CE	LYS E			51.521	14.99		245.72
,	3341	NZ	LYS B			55.806	11.22	7 1.00	236.74
	3342	С	LYS B			56.797	11.84		236.74 197.18
	3343	0	LYS B	_	8 32.415 9 31.805	55.821	9.92		197.18
	3344	N	TRP 8	_	9 31.948	57.042	9.14		174.88
•	3345	CA	TRP B	_	39 33.131	56. 9 37	8.18		174.88
	3346	CB CC	TRP E	_	39 34.474	56.888	8.84		174.88
	3347	CD2			39 35.068	57.877	9.70		174.88
	3348	CE2			39 36.391		9.97 10.27		174.88
	3349	CE3			39 34.614		8.6		174.88
(65 3350 3351	CD1		в :	39 35.433		9.3		174.88
	3351	NE1	TRP !	в :	39 36.589		10.7	• •	174.88
	3353	CZ2	TRP	_	39 37.265		11.0	82 1.00	
	3354	CZ3			39 35.484 39 36.79		11.3		174.88
	70 3355	CH2	TRP	ø	39 36.79	50.031	•		

		_	TOD 8	39.	30.667	57.211	8.335	1.00	197.18
	3356	C		39	30.215	56.251	7.708	1.00	197.18
	3357	0	TRP B PHE B	40	30.086	58.413	8.348	1.00	196.05 196.05
	3358	N CA	PHE B	40	28.848	58.653	7.609	1.00 1.00	216.66
_	3359	CB	PHE B	40	27.674	58.878	8.572	1.00	216.66
5	3360	CG	PHE B	40	27.425	57.738	9.528 10.679	1.00	216.66
	3361 3362	CD1	PHE B	40	28.199	57.602	9.297	1.00	216.66
	3363	CD2	PHE B	40	26.396	56.824 56.578	11.590	1.00	216.66
	3364	CE1	PHE B	40	27.951	55.800	10.194	1.00	216.66
10	3365	CE2	PHE B	40	26.139 26.917	55.674	11.345	1.00	216.66
10	3366	CZ	PHE B	40	28.896	59.825	6.616	1.00	196.05
	3367	С	PHE B	40 40	28.336	60.888	6.877	1.00	196.05
	3368	0	PHE B HIS B	41	29.552	59.613	5.476	1.00	132.87
	3369	N	HIS B HIS B	41	29.665	60.618	4.418	1.00	132.87 148.70
15	3370	CA CB	HIS B	41	30.576	60.097	3.315	1.00 1.00	148.70
	3371	CG	HIS B	41	30.772	61.067	2.198	1.00	148.70
	3372	CD2	HIS B	41	30.886	60.877	0.864 2.414	1.00	148.70
	3373	ND1	HIS B	41	30.949	62.416	1.259	1.00	148.70
20	3374 3375	CE1	HIS B	41	31.166	63.019	0.304	1.00	148.70
20	3376	NE2	HIS B	41	31.135	62.108 60.975	3.804	1.00	132.87
	3377	С	HIS B	41	28.311	60.210	2.996	1.00	132.87
	3378	0	HIS B	41	27.783	62.147	4.163	1.00	209.30
	3379	N	ASN B	42	27.777 26.467	62.614	3.684	1.00	209.30
25	3380	CA	ASN B	42	26.371	62.546	2.148	1.00	240.31
	3381	CB	ASN B	42 42	27.092	63.700	1.461	1.00	240.31
	3382	CG	ASN B ASN B	42	28.241	63.989	1.789	1.00	240.31 240.31
	3383	OD1	ASN B	42	26.427	64.350	0.505	1.00	209.30
	3384	ND2	ASN B	42	25.375	61.745	4.316	1.00 1.00	209.30
30	3385	CO	ASN B	42	24.271	61.613	3.774 5.475	1.00	171.14
	3386 3387	Ň	GLY B	43	25.695	61.168	6,176	1.00	171.14
	3388	ĞA	GLY B	43	24.758	60.306	5.841	1.00	171.14
	3389	C	GLY B	43	24.985	58.836 57.969	6.717	1.00	171.14
35	3390	0	GLY B	43	24.963	58.563	4.560	1.00	214.62
55	3391	N	SER B	44	25.211 25.444	57.207	4.071	1.00	214.62
	3392	CA	SER B	44 44	25.676	57.228	2.555	1.00	249.69
	3393	CB	SER B	44	24.567	57.774	1.864	1.00	249.69 214.62
40	3394	OG	SER B SER B	44	26.651	56.559	4.733	1.00 1.00	214.62
40	3395	CO	SER B	44	27.757	57.088	4.657	1.00	180.32
	3396	N	LEU B	45	26.448	55.404	5.359 6.008	1.00	180.32
	3397 3398	CA	LEU B	. 45	27.555	54.713	6.558	1.00	218.81
	3399	СВ	LEU B	45	27.095	53.361 52.573	7.318	1.00	218.81
45		CG	LEU B	45	28.170	53.429	8.432	1.00	218.81
45	3401	CD1	LEU B	45	28. 75 3 27.568	51.300	7,883	1.00	218.81
	3402	CD2	LEU B	45		54.516	5.030	1.00	180.32
	3403	Ç	LEU B	45 45		54.379	3.819		180.32
	3404	0	LEU B SER B	46		54.517	5.565		248.98 248.98
50		N	SER B	. 46		54.357	4.757		249.38
	3406	CA CB	SER B	46	32.188	55.405	5.149 4.301		249.38
	3407	OG OG	SER B	46	33.322	55.338	4.898		248.98
	3408 3409	č	SER B	46		52.967	5.773		248.98
5	5 3410	ŏ	SER B			52.195 52.670	4.04		249.69
J.	3411	N	GLU B			51.365	4.03		249.69
	3412	CA	GLU B			50.996	2.59		249.69
	3413	СВ	GLU B		7 33. 7 57 32.553	50.869	1.67	4 1.00	249.69
	3414	CG	GLU B		·	50.524	0.25		249.69
6	0 3415	CD	GLU B		7 32.945 7 33.631	51.350	-0.38		249.69 249.69
	3416	OE1	GLU E		7 32.572	49.426	-0.21		249.69
	3417	OE2	GLU E		7 34.618	51.211	4.92		249.69
	3418	C	GLU E	-	7 35.099	50.096	5.13		184.88
	3419	0 N	GLU (-	48 35.139	52.316	5.44 6.31		184.88
•	55 3420	CA	GLU I	-	48 36.297		6.2		208.21
	3421 3422	. CB	GLU I	В 4	48 37.110		7.20		208.21
	3423	CG	GLU	В	48 38.293		6.9		208.21
	3424	CD	GLU	В	48 39.366		5.9		208.21
•	70 3425	OE1	GLU	В	48 40.084	, 32,000	3		

	0.400	OE2	GLU B	48 .	39,493	51.517	7.685	1.00	208.21
	3426		GLU B	48	35.834	51.929	7.738	1.00	184.88
	3427	C			34.687	52.213	8.104	1.00	184.88
	3428	0	GLU B	48		51.348	8.530	1.00	237.20
_	3429	N	THR B	49	36.731	51,003	9.917	1.00	237.20
5	3430	CA	THR B	49	36.443		10.090	1.00	231.33
	3431	СВ	THR B	49	36.348	49.477	9.586	1.00	231.33
	3432	OG1	THR B	49	37.542	48.864			
	3433	CG2	THR B	49	35.144	48.933	9.336	1.00	231.33
	3434	С	THR B	49	37.540	51,551	10.829	1.00	237.20
10	3435	0	THR B	49	37.303	51.819	12.006	1.00	237.20
	3436	N	ASN B	50	38.739	51.713	10.278	1.00	222.02
	3437	CA	ASN B	50	39.863	52.246	11.036	1.00	222.02
	3438	CB	ASN B	50	41.101	52.350	10.132	1.00	245.81
	3439	ĊĠ	ASN B	50	42.369	52.650	10.910	1.00	245.81
15	3440	OD1	ASN B	50	42.309	53.119	12.045	1.00	245.81
13	3441	ND2	ASN B	50	43.520	52.400	10.299	1.00	245.81
	3442	C	ASN B	50	39.447	53.636	11.531	1.00	222.02
		ŏ	ASN B	50	38.625	54.290	10.901	1.00	222.02
	3443	N	SER B	51	40.004	54.089	12.651	1.00	208.27
20	3444	ČA	SER B	51	39.652	55.405	13.176	1.00	208.27
20	3445		SER B	51	40.219	55.590	14.590	1.00	249.69
	3446	CB			41.624	55.785	14.565	1.00	249.69
	3447	og	SER B	51	40.135	56.555	12.276	1.00	208.27
	3448	Ç	SER B	51		57.690	12.416	1.00	208.27
~ ~	3449	0	SER B	51	39.672		11.360	1.00	249.32
25	3450	N	SER B	52	41.059	56.265		1.00	249.32
	3451	CA	SER B	52	41.588	57.283	10.446		
	3452	CB	SER B	52	43.125	57.283	10.456	1.00	193.43
	3453	OG	SER B	52	43.642	57.584	11.741	1.00	193.43
	3454	С	SER B	52	41.106	57.076	9.014	1.00	249.32
30	3455	0	SER B	52	41.596	56.199	8.299	1.00	249.32
•	3456	N	LEU B	53	40.147	57.895	8.601	1.00	187.33
	3457	CA	LEU B	53	39,601	57.820	7.255	1.00	187.33
	3458	CB	LEU B	53	38.107	58.131	7.283	1.00	113.92
	3459	CG	LEU B	53	37.410	58.539	5.975	1.00	113.92
35	3460	CD1	LEU B	53	37.839	57. 63 7	4.810	1.00	113.92
J	3461	CD2	LEU B	53	35.889	58.503	6.185	1.00	113.92
	3462	C	LEU B	53	40.310	58.794	6.331	1.00	187.33
	3463	ŏ	LEU B	53	40.085	60.010	6.397	1.00	187.33
	3464	Ň	ASN B	54	41.169	58.261	5.467	1.00	190.27
40	3465	ĊA	ASN B	54	41.899	59.112	4.547	1.00	190.27
70	3466	CB	ASN B	54	43,209	58.458	4.126	1.00	248.26
	3467	CG	ASN B	54	44.214	58.414	5.254	1.00	248.26
		OD1	ASN B	54	44.519	59.432	5.876	1.00	248.26
	3468	ND2	ASN B	54	44.737	57.232	5.525	1.00	248.26
45	3469		ASI: B	54	41.096	59.481	3,320	1.00	190.27
45	3470	C	ASN B	54	40.134	58.800	2.957	1.00	190.27
	3471	0	ILE B	55	41.515	60.580	2.700	1.00	195.13
	3472	N	ILE B	55	40.900	61.127	1.503	1.00	195.13
	3473	CA		55	40.101	62.413	1.829	1.00	126.27
50	3474	CB		55	39.946	63.268	0.581	1.00	126.27
50	3475	CG2	ILE B			62.032	2.431	1.00	126.27
	3476	CG1	ILE B	55	38.743	63.206	2.786	1.00	120.27
	3477	CD1	ILE B	55	37.857	61.473	0.540	1.00	195.13
	3478	Ç	ILE B	55	42.017		0.825	1.00	195.13
	3479	0	ILE B	55	42.836	62.346		1.00	178.85
55	3480	N	VAL B	56	42,057	60.789	-0.594 -1.569	1.00	178.85
	3481	CA	VAL B	56	43.099	61.058			249.69
	3482	CB	VAL B	56	43.587	59.773	-2.227	1.00	249.69
	3483	CG1	VAL B	56	44.960	60.002	-2.841	1.00	
	3484	CG2	VAL B	56	43.642	58.662	-1.189	1.00	249.69
60	3485	С	VAL B	56	42.580	62.012	-2.630	1.00	178.85
	3486	0	VAL B	56	41.612	62.729	-2.376	1.00	178.85
	3487	N	ASN B	57	43.217	62.025	-3.804	1.00	192.84
	3488	CA	ASN B	57	42.832	62.923	-4.895	1.00	192.84
	3489	СВ	ASN B	57	43.085	62.261	-6.239	1.00	201.25
65	3490	CG	ASN B	57	44.560	62.119	-6.530	1.00	201.25
55	3491	OD1	ASN B	57	45.309	63.090	-6.448	1.00	201.25
	3492	ND2	ASN B	57	44.988	60.908	-6.875	1.00	201.25
	3493	C	ASN B	57	41.397	63.405	-4.791	1.00	192.84
	3494	ŏ	ASN B	57	40.470	62.757	-5.267	1.00	192.84
70	3495	Ň	ALA B	58	41.253	64.565	-4.151	1.00	127.65
70	J-100	••							

						65.227	-3.870	1.00	127.65
	3496	CA		-	9.980	66.555	-3.201	1.00	133.74
	3497	СВ	/ Was 1 -	•	0.256	65.436	-5.041	1.00	127.65
	3498	С	, . . –	-	19.029 19.244	66.294	-5.891	1.00	127.65
	3499	0	,		37.956	64.658	-5.060	1.00	124.63
5	3500	N			36.946	64.744	-6.109	1.00	124.63
_	3501	CA	LYS B Lys b		36.504	63.344	-6.550	1.00	240.20 240.20
	3502	CB	LYS B		37.632	62.491	-7.108	1.00 1.00	240.20
	3503	CD	LYS B	59	37.182	61.069	-7.421 -7.901	1.00	240.20
10	3504	CE	LYS B		38.354	60.214	-8.237	1.00	240.20
10	3505 3506	NZ	LYS B		37.959	58.816 65.493	-5.511	1.00	124.63
	3507	Ċ	LYS B		35.778	65.278	-4.355	1.00	124.63
	3508	0	LYS B		35.423 35.188	66.378	-6.301	1.00	146.51
	3509	N	PHE B	•-	34.064	67.179	-5.839	1.00	146.51
15	3510	CA	PHE B PHE B	60 60	33.350	67.788	-7.049	1.00	206.05 206.05
	3511	CB	PHE B	60	34.189	68.770	-7.815	1.00 1.00	206.05
	3512	CG	PHE B	60	33.968	68.976	-9.169	1.00	206.05
	3513	CD1 CD2	PHE B	60	35.193	69.499	-7.177 -9.882	1.00	206.05
20	3514	CE1	PHE B	60	34.732	69.890	-7.877	1.00	206.05
20	3515 3516	CE2	PHE B	60	35.963	70.417 70.612	-9.234	1.00	206.05
	3517	CZ	PHE B	60	35.732	66.407	-4.968	1.00	146.51
	3518	С	PHE B	60	33.073 32.479	66.957	-4.044	1.00	146.51
	3519	0	PHE B	60	32.911	65.125	-5.257	1.00	158.05
25	3520	N	GLU B	61 61	31.977	64.284	-4.520	1.00	158.05 249.69
	3521	CA	GLU B	61	31.872	62.911	-5.197	1.00	249.69
	3522	CB	GLU B	61	31.394	62.950	-6.651	1.00 1.00	249.69
	3523	CG CD	GLU B	61	32.288	63.798	-7.556 -7.574	1.00	249.69
20	3524	OE1	GLU B	61	33.522	63.580	-7.574 -8.256	1.00	249.69
30	3525 3526	OE2	GLU B	61	31.753	64.685 64.113	-3.067	1.00	158.05
	3527	C	GLU B	61	32.391	63.831	-2.213	1.00	158.05
	3528	0	GLU B	61	31.555 33.682	64.285	-2.789	1.00	134.92
	3529	N	ASP B	62 62	34.200	64.139	-1.426	1.00	134.92 133.92
35	3530	CA	ASP B	62	35.729	64.128	-1.432	1.00	133.92
	3531	CB	ASP B ASP B	62	36.294	63.118	-2.393	1.00 1.00	133.92
	3532	CG OD1	ASP B	62	35.669	62.048	-2.551 -2.972	1.00	133.92
	3533	OD2	ASP B	62	37.364	63.397	-0.543	1.00	134.92
40	3534) 3535	C	ASP B	62	33.709	65.279 65.143	0.685	1.00	134.92
40	3536	Ŏ	ASP B	62	33.663	66.400	-1.177	1.00	128.21
	3537	N	SER B	63	33.358 32.857	67.553	-0.449	1.00	128.21
	3538	CA	SER B SER B	63 63	32.552	68.710	-1.407	1.00	212.43 212.43
	3539	CB	SER B	63	33.696	69.095	-2.153	1.00 1.00	128.21
4:		C C	SER B	63	31.574	67.137	0.261 -0.377	1.00	128.21
	3541	ŏ	SER B	63	30.660	66.629	1.571	1.00	137.99
	3542 3543	Ň	GLY B	64	31.500	67.347 68.963	2.274		137.99
	3544	CA	GLY B	64	30.298	66.973	3.784	1.00	137.99
5	0 3545	C	GLY B	64	30. 367 31. 282	67.545	4.385		137.99 125.38
_	3546	0	GLY B	64 65	29.378	66.312	4.383		125.38
	3547	N	GLU B GLU B	65	29.219	66.217	5.830		249.57
	3548	CA	GLU B		27.747	66.504	6.159 7.594		249.57
	3549	CB	GLU B	65	27.329	66.290	7.5 5 7.73		249.57
	55 3550 3551	CD	GLU B	65	25.818	66.198 65.270	7.14		249.57
	3552	OE1	GLU B	65		67.046	8.41	6 1.00	249.57
	3553	OE2	GLU B	65		64.843	6.33	9 1.00	125.38
	3554	С	GLU B			63.844	5.90		125.38 138.71
	60 3555	0	GLU E			64,790	7.26		138.71
	3556	N	TYR E			63.510	7.82		186.43
	3557	CA	TYR			63.294	7.56		186.43
	3558	CB	TYR		32.917	63.170	6.12 5.30		186.43
	3559 65 3560	CD1	TYR I	B 60		64.287	3.9		186.43
	3561	CE1	TYR !	B 64		64.189 61.943	5.6		186.43
	3562	CD2	TYR	B 6		61.827	4.3	14 1.00	186.43
	3563	CE2	TYR			62.957	3.5		186.43
	3564	CZ	TYR		6 33.871 6 34.375		2.2	20 1.00	186.43
	70 3565	OH	TYR	,					

		С	TYR B	66 [°]	30.823	63.378	9.345 10.022	1.00 1.00	138.71 138.71
	3566	ŏ	TYR B	66	30.510	64.370 62.155	9.862	1.00	179.70
	3567 3568	N .	LYS B	67	31.029	61.847	11.295	1.00	179.70
	3569	CA	L	67	30.895	62.047	11.754	1.00	159.69
5	3570	CB	LYS B	67	29.456	61.317	10.919	1.00	159.69
5	3571	CG	LYS B	67	28.447 27.057	61.654	11.392	1.00	159.69
	3572	CD	LYS B	67	26.005	61.334	10.324	1.00	159.69
	3573	CE	LYS B	67 67	24.591	61,613	10.773	1.00	159.69
	3574	NZ	LYS B	67	31.323	60.434	11.691	1.00	179.70 179.70
10	3575	C	LYS B Lys b	67	31.284	59.505	10.885	1.00 1.00	162.03
	3576	0	CYS B	68	31.723	60.285	12.953	1.00	162.03
	3577	N	CYS B	68	32.142	58.993	13.489	1.00	162.03
	3578	CA	CYS B	68	31.445	58.691	14.810 15.578	1.00	162.03
	3579	C O	CYS B	68	31.102	59.589	13.665	1.00	220.63
15	3580	СВ	CYS B	68	33.670	58.915	14.951	1.00	220.63
	3581	SG	CYS B	68	34.426	59.969 57.402	15.049	1.00	249.69
	3582 3583	N	GLN B	69	31.239	56.906	16.245	1.00	249.69
	3584	CA	GLN B	69	30.573	56.763	15.965	1.00	222.67
20	3585	СВ	GLN B	69	29.078	55.832	16.904	1.00	222.67
20	3586	CG	GLN B	69	28.343 26.898	55.619	16.496	1.00	222.67
	3587	CD	GLN B	69	26.612	55.268	15.351	1.00	222.67
	3588	OE1	GLN B	69	25.977	55.823	17.435	1.00	222.67 249.69
	3589	NE2	GLN B	69 69	31.168	55.546	16.606	1.00	249.69
25	3590	Ç	GLN B	69	31.580	54.788	15.727	1.00	249.63
	3591	0	GLN B HIS B	70	31.219	55.235	17.897	1.00 1.00	249.63
	3592	N	HIS B HIS B	70	31.762	53.956	18.331	1.00	248.69
	3593	CA	HIS B	70	32.637	54.139	19.570 19.289	1.00	248.69
	3594	CB CG	HIS B	70	33.932	54.841	19.864	1.00	248.69
30	3595	CD2	HIS B	70	34.500	55.925	18.304	1.00	248.69
	3596	ND1	HIS B	70	34.798	54.422 55.223	18.283	1.00	248.69
	3597 3598	CE1	HIS B	70	35.852	56.141	19.217	1.00	248.69
	3599	NE2	HIS B	70	35.696	52.952	18.618	1.00	249.63
35	3600	C	HIS B	70	30.656 29.488	53.196	18.308	1.00	249.63
73	3601	0	HIS B	70	31.032	51.824	19.211	1.00	249.69 249.69
	3602	N	GLN B	71 71	30.087	50.755	19.541	1.00	249.69
	3603	CA	GLN B GLN B	71	30.836	49.613	20.251	1.00	249.69
	3604	CB	GLN B	71	30.136	48.247	20.254	1.00 1.00	249.69
40	3605	CG	GLN B	71	29.921	47.672	18.850 18.016	1.00	249.69
	3606	CD	GLN B	71	30.834	47.657	18.594	1.00	249.69
	3607	OE1 NE2	GLN B	71	28.710	47.183	20.410	1.00	249.69
	3608	C	GLN B	71	28.923	51.253	20.118	1.00	249.69
44	3609	ŏ	GLN B	71		50.990 51.983	21.471	1.00	249.69
4:	5 3610 3611	Ň	GLN B	72		52.506	22.371	1.00	249.69
	3612	CA	GLN B	72		51.678	23.671	1.00	249.69
	3613	CB	GLN B	72		52.118	24.772	1.00	249.69
	3614	CG	GLN B	72		51.390	26.084		249.69 249.69
5	0 3615	CD	GLN B	72 72		50.159	26.130		249.69
_	3616	OE1	GLN B	7		52.151	27.156		249.69
	3617	NE2	GLN B			53.997	22.656		249.69
	3618	C	GLN B			54.423	23.809 21.588		249.69
	3619	0	VAL B		3 28.533	54.787	21.718		249.69
5	5 3620	N	VAL B		3 28.747	56.226	21.45	-	227.88
	3621	CA CB	VAL B		3 30.224	56.626	21.91		227.88
	3622	CG1	VAL E		3 30.454	58.055	22.17		227.88
	3623	CG2	VAL E		31.167		20.69		249.69
	3624 60 3625	Č	VAL E	3 7	73 27.875	440	19.57		249.69
,	3626	ŏ	VAL E		73 27.681		21.06		249.69
	3627	Ň	ASN E	-	74 27.348		20.15	6 1.00	249.69
	3628	CA	ASN	_	74 26.504 74 25.675		20.95		218.87
	3629	CB	ASN 1				22.05		218.87
	65 3630	CG	ASN	_	74 24.852 74 24.270		21.84		218.87 218.87
	3631	OD1		_	74 24.79		23.2		218.67
	3632	ND2	ASN	_	74 27.36	8 59.564	19.10		249.69
	3633	C	ASN ASN	Б	74 28.34	2 60.240	19.4		242.43
	3634	0 7	GLU		75 27.00		17.8		
	70 3635	14	G_5 0	-	•				

							40.704	1.00	242.43
	3636	CA	GLU B	75 ⁻	27.735	59.968	16.704 15.429	1.00	240.14
	3637	CB	GLU B	75	26.889	59.853	15.649	1.00	240.14
	3638	CG	GLU B	75	25.394	60.044 59.681	14.423	1.00	240.14
	3639	CD	GLU B	75	24.571	58.580	13.867	1.00	240.14
5	3640	OE1	GLU B	75 75	24.782 23.709	60.493	14.021	1.00	240.14
_	3641	OE2	GLU B	75 75	28.199	61.410	16.900	1.00	242.43
	3642	Ç	GLU B	75 75	27.478	62.241	17.453	1.00	242.43
	3643	0	GLU B SER B	76	29.413	61.690	16.427	1.00	249.69
10	3644	N CA	SER B	76	30.030	63.012	16.552	1.00 1.00	249.69 193.15
10	3845	CB	SER B	76	31.491	62.960	16.091	1.00	193.15
	3646 3647	OG	SER B	76	31.574	62.865	14.681 15.766	1.00	249.69
	3648	Č	SER B	76	29.323	64.104 63.825	14.813	1.00	249.69
	3649	0	SER B	76	28.595	65.351	16.175	1.00	227.37
15	3650	N	GLU B	77	29.555 28.9 6 9	66.496	15.500	1.00	227.37
	3651	CA	GLU B	77 77	29.300	67.790	16.252	1.00	249.69
	3652	CB	GLU B GLU B	77	28.667	67.874	17.635	1.00	249.69
	3653	cg	GLU B	77	27.144	67.885	17.588	1.00	249.69 249.69
20	3654	OE1	GLU B	77	26.566	67.679	16.493	1.00 1.00	249.69
20	3655 3656	OE2	GLU B	77	26.521	68.094	18.654 14.099	1.00	227.37
	3657	C	GLU B	77	29.556	66.554	13.926	1.00	227.37
	3658	ŏ	GLU B	77	30.747	66.802 66.324	13.072	1.00	151.66
	3659	N	PRO B	78	28.708	66.271	13,163	1.00	139.99
25	3660	CD	PRO B	78 70	27.233 29.168	66.339	11.671	1.00	151.66
	3661	CA	PRO B	78 78	27.852	66,486	10.892	1.00	139.99
	3662	CB	PRO B PRO B	78	26.833	65.808	11.784	1.00	139.99
	3663	CG	PRO B	78	30.136	67.473	11.369	1.00	151.66 151.66
20	3664	C	PRO B	78	30.182	68.466	12.086	1.00 1.00	174.84
30	3665 3666	N	VAL B	79	30.929	67.306	. 10.321 9.905	1.00	174.84
	3667	CA	VAL B	79	31.855	68.352	10.222	1.00	152.46
	3668	СВ	VAL B	79	33.336	68.021 69.029	9.536	1.00	152.46
	3669	CG1	VAL B	79	34.256 33.566	68.076	11.714	1.00	152.46
35	3670	CG2	VAL B	79 79	31.682	68.435	8.405	1.00	174.84
	3671	Ç	VAL B	79	31.482	67.408	7.752	1.00	174.84
	3672	0	VAL B TYR B	80	31.738	69.642	7.850	1.00	124.58 124.58
	3673	N GA	TYR B	80	31.564	69.771	6.414	1.00 1.00	201.47
40	3674 3675	CB	TYR B	80	30.573	70.877	6.084 4.675	1.00	201.47
40	3676	CG	TYR B	80	30.044	70.777 69.936	4.370	1.00	201.47
	3677	CD1	TYR B	80	28.979	69.801	3.072	1.00	201.47
	3678	CE1	TYR B	80		71.484	3.641	1.00	201.47
0.2	3679	CD2	TYR B	80 80		71.356	2.334	1.00	201.47
45		CE2	TYR B TYR B	80		70.514	2.057	1.00	201.47 201.47
•	3681	CZ OH	TYR B	80		70.383	0.762	1.00 1.00	124.58
	3682 3683	Ċ	TYR B	80	32.861	70.049	5.704 6.140	1.00	124.58
	3684	ŏ	TYR B	80		70.887	4.606	1.00	114.91
50	3685	N	LEU B	81		69.344 69.544	3.839	1.00	114.91
•	3686	CA	LEU B	81		68.223	3.661	1.00	104.59
	3687	CB	LEU B	81 81		68.327	2.720		104.59
	3688	ca	LEU B	8		69.306	3.327		104.59 104.59
_	3689	CD1 CD2	LEU B	8		66.972	2.487		114.91
5	5 3890 3891	C	LEU B	8	1 33.917	70.087	2,482 1,836		114.91
	3692	ŏ	LEU B	8		69.517	2.049		120.70
	3693	N	GLU B			71.184 71. 73 4	0.725		120.70
	3694	CA	GLU B		2 34.244 2 33.716	73.163	0.833		201.66
6	0 3695	CB	GLU B	. 8	2 33.716 2 32.820	73.551	-0.332		201.66
	3696	ÇG	GLU B		32.280	74.954	-0.21		201.66 201.66
	3697	CD	GLU B		32.022	75.401	0.92		201.66
	3698	OE1 OE2	GLU E		32 32,100	75.610	-1.26		120.70
	3699 55 3700	C	GLU E	-	35.482	71.691	-0.17		120.70
,	3700 3701	ŏ	GLU E	3 1	82 38.583	72.004	0.27 -1.43		157.10
	3702	Ň	VAL E	3	83 35.299	71.276 71.204	-2.39	_	157.10
	3703	CA	VAL	_	83 36.398		-3.03	1.00	142.28
	3704	СВ	VAL		83 36.519 83 37.699		-4.00		142.28
,	70 3705	CG1	VAL	_	,	•			

						68.770	-1.955	1.00	142.28
	3706	CG2	4114 -	83	36.708	72.239	-3.494	1.00	157.10
	3707	C	AVE -	83	36.227 35.120	72,455	-3.992	1.00	157.10
	3708	0		83	37.344	72.845	-3.895	1.00	122.91
	3709	N	PHE B	84 84	37.331	73.921	-4.875	1.00	122.91 156.44
5	3710	CA	PHE B PHE B	84	37.654	75.240	-4.180 0.406	1.00 1.00	156.44
	3711	CB	PHE B	84	36.687	75.629	-3.106 -1.821	1.00	156.44
	3712	CG	PHE B	84	36.773	75.093	-3.382	1.00	156.44
	3713	CD1 CD2	PHE B	84	35.696	76.562 75.485	-0.833	1.00	156.44
10	3714	CE1	PHE B	84	35.885	76.958	-2.401	1.00	156.44
10	3715 3716	CE2	PHE B	84	34.805	76.419	-1.121	1.00	156.44
	3717	CZ	PHE B	84	34.903 38.259	73.854	-6.045	1.00	122.91
	3718	C	PHE B	84	39,300	73.198	-6.007	1.00	122.91 152.63
	3719	0	PHE B	84 85	37.884	74.614	-7.064	1.00	152.63
15	3720	N	SER B SER B	85	38.690	74.765	-8.267	1.00 1.00	143.15
	3721	CA	SER B	85	38.054	74.080	-9.467 -10.617	1.00	143.15
	3722	CB OG	SER B	85	38.872	74.255	-8.523	1.00	152.63
	3723	C	SER B	85	38.741	76.262	-8.796	1.00	152.63
20	3724	ŏ	SER B	85	37.715	76.882 76.836	-8.412	1.00	139.36
20	3725 3726	Ň	ASP B	86	39.933	78.263	-8.613	1.00	139.36
	3727	CA	ASP B	86	40.120	79.047	-7.577	1.00	172.94
	3728	СВ	ASP B	86	39.314 38.724	80.313	-8.143	1.00	172.94 172.94
	3729	CG	ASP B	86 86	39.476	81.114	-8.744	1.00	172.94
25	3730	OD1	ASP B	86	37.505	80.511	-7.977	1.00 1.00	139.36
	3731	OD2	ASP B ASP B	86	41.606	78.609	-8.458 -7.963	1.00	139.36
	3732	C	ASP B	86	42.379	77.794	-7.963 -8.863	1.00	121.62
	3733	0 N	TRP B	87	42.003	79.814	-8.745	1.00	121.62
20	3734	CA	TRP B	87	43.393	80.224 81.544	-9,459	1.00	247.13
. 30	3735 3736	CB	TRP B	87	43.617	81.344	-10.891	1.00	247.13
	3737	CG	TRP B	87	43.989 43.103	81.328	-12.013	1.00	247.13 247.13
	3738	CD2	TRP B	87 87	43.881	81.063	-13.164	1.00	247.13
	3739	CE2	TRP B	87		81.521	-12.166	1.00 1.00	247.13
35	3740	CE3	TRP B	87		81.085	-11.386 -12.752	1.00	247.13
	3741	CD1 NE1	TRP B	87		80.918	-14.445	1.00	247.13
	3742	CZ2	TRP B	87	43.328	80.982	-13.443	1.00	247.13
	3743 3744	CZ3	TRP B	87		81.442 81.171	-14.563	1.00	247.13
40		CH2	TRP B	87		80.336	-7.288	1.00	121.62
40	3746	С	TRP B	87		79.726	-6.870	1.00	121.62 133.11
	3747	0	TRP B	87 88		81.106	-6.510		133.11
	3748	N	LEV B	8		81.246	-5.092 -4.789		136.45
	3749	CA	LEU B	8	8 43.787	82.678	-4.768 -5.444		130.45
45	3750	CB	LEU B	8	8 45.105	83.123	-4.973		136.45
	3751	CD1	LEU B		8 45.489	84.525 82.131	-5.093	3 1.00	136.45
	3752 3753	CD2	LEU B		18 46.196 18 42.137	80.876	-4.219	3 1.00	133.11
	3754	С	LEU B			81.159	-4.57		133.11 126.96
5	0 3755	0	LEU B		38 40.985 39 42.413	80.222	-3.08		126.96
	3756	N	LEU B		89 41.363	79.834	-2.14		166.49
	3757	CA	LEU B		89 41.152		-2.15 -1.13		166.49
	3758	CB CG	LEU B		89 40.113		-1.30		156.49
_	3759	CD1	LEU E	3	89 38.812		-1.30	00 1.00	(38.49
2	5 3760 3761	CD2	LEU E	3	89 39.881		-0.74	1.00	126.96
	3762	Ċ	LEU	-	89 41.777 89 42.900	70 070	-0.33		126.96 113.68
	3763	0	LEU		90 40.883		-0.0		113.68
	3764	N	LEU (90 41.196	3 81.391	1.3		125.93
(60 3765	CA	LEU		90 40.42	2 82.674	1.6 3.1		125.93
	3766	CB CG	LEU		90 40.53	6 83.133	3.1		125.93
	3767	CD1		В	90 41.98	A 4 070	3.3		125.93
	3768	CD	. LEU	В	90 39.69		2.3	56 1.00	113.68
	3769 65 3770	c c	LEU	В	90 40.85			66 1.00	113.68
	3771	ŏ	LEU	В	90 39.69 91 41.87			1.00	
	3772	N	GLN	В	91 41.87 91 41.64	70 704		000 1.00	4-4 07
	3773			D R	91 42.60	77.614	•	842 1.00 481 1.00	
	3774				91 42.6		. 2.	481 1.00	
	70 3775	CG	,	-					

							0.262	1.00	171.07
		CD	GLN B	91 [*]	43.685	75.865	2.363 2.555	1.00	171.07
	3776	OE1	GLN B	91	44.878	76.095 74.660	2.046	1.00	171.07
3	3777 3778	NE2	GLN B	91	43.232	79.237	5.422	1.00	98.97
	3779 3779	Ċ.		91	41.707 42.592	80.023	5.780	1.00	98.97
	3780	0	GLN B	91 92	40.769	78.773	6.244	1.00	123.57 123.57
	3781	N	ALA B ALA B	92	40.707	79.189	7.645	1.00 1.00	155.46
	3782	CA CB	ALA B	92	39.422	79.967	7.914 8.537	1.00	123.57
	3783	C	ALA B	92	40.774	77.974	8.208	1.00	123.57
	3784	ŏ	ALA B	92	40.215	76.918 78.126	9.662	1.00	119.49
10	3785 3786	N	SER B	93	41.473	77.046	10.652	1.00	119.49
	3787	CA	SER B	93	41.631 42.377	77.561	11.897	1.00	144.43
	3788	CB	SER B	93 9 3	41.794	78.730	12.443	1.00	144.43 119.49
	3789	og .	SER B	93	40.238	76.547	11.026	1.00 1.00	119.49
15	3790	CO	SER B	93	39.891	75.389	10.783 11.605	1.00	139.25
	3791	N	ALA B	94	39.447	77.448 77.173	11.989	1.00	139.25
	3792 3793	ĞA	ALA B	94	38.072	77.053	13.497	1.00	173.88
	3794	CB	ALA B	94	37.961 37.289	78.378	11.484	1.00	139.25
20	3795	С	ALA B	94 94	37.843	79.465	11.346	1.00	139.25 153.31
20	3796	0	ALA B GLU B	95	36.010	78.197	11.188	1.00 1.00	153.31
	3797	N	GLU B	95	35.217	79.312	10.694 9.648	1.00	193.17
	3798	CA CB	GLU B	95	34.219	78.813	8.419	1.00	193.17
05	3799	CG	GLU B	95	34.894	78.235 77.974	7.284	1.00	193.17
25	3800 3801	CD	GLU B	95	33.929	77.478	6.230	1.00	193.17
	3802	QE1	GLU B	95	34.372 32.727	78.269	7.442	1.00	193.17 153.31
	3803	OE2	GLU B	95 95	34.493	80.058	11.817	1.00	153.31
	3804	Č	GLU B	95	34.153	81.241	11.678	1.00 1.00	119.30
30	3805	0	VAL B	96	34.272	79.364	12.930 14.087	1.00	119.30
	3806	N CA	VAL B	96	33.599	79.942	14.355	1.00	135.82
	3807 3808	CB	VAL B	96	32.262	79.239 80.129	15.250	1.00	135.82
	3809	CG1	VAL B	96	31.387 31.566	78.905	13.045	1.00	135.82
35	3810	CG2	VAL B	96	34.482	79.788	15.330	1.00	119.30 119.30
55	3811	C	VAL B	96 96	34.967	78.690	15.622	1.00 1.00	139.44
	3812	0	VAL B VAL B	97	34.664	80.871	16.082 17.247	1.00	139.44
	3813	N GA	VAL B	97		80.799	16.927	1.00	116.73
40	3814	CB	VAL B	97		81.401 80.880	17.910		116.73
40	3815 3816	CG1	VAL B	97		81.074	15.506	1.00	116.73
	3817	CG2	VAL B	97		81.451	18.543		139.44 139.44
	3818	C	VAL B	97 97		82.445	18.528		148.58
	3819	0	VAL B MET B	91		80.882	19.659		148.58
45	3820	N CA	MET B	9	35.228	81.363	21.015 22.03		249.69
	3821	CB	MET B	9		80.224 79.059	21.89		249.69
	3822 3823	ÇĞ	MET B	9		79.444	22.53	1 1.00	249.69
	3824	SD	MET B		8 32.799 8 33.078	79.331	24.29		249.69 148.58
50	0 3825	CE	MET B		8 33.078 8 36.217	82.467	21.36		148.58
_	3826	C	MET B		8 37.425	82.250	21.30		152.43
	3827	O N	GLU B		9 35.721	83.636	21.75 22.10		152.43
	3828	CA	GLU B	, ,	9 38.604		22.97		244.45
<	3829 5 3830	ČĽ.	GLU E	3 9	99 35.865		22.89	1.00	244.45
J	3831	CG	GLU E		99 36.447 99 35.891	** ***	23.9		244.45 244.45
	3832	CD	GLU E	-	99 35.891 99 34.681		24.2		244.45
	3833	OE1			99 36.66	88.930	24.4		152.43
	3834	OE2	GLU	B	99 37.83	84.264	22.8 23.8		152.43
•	50 3835	C	GLU.	_	99 37.70		22.3		146.37
	3836 3837	Ň	GLY	В	100 39.01		23.0	53 1.00	146.37
	3838	CA	GLY	В	100 40.21		22.3	1.00	
	3839	C	GLY	В	100 41.00 100 42.20	~	22.0		
4	65 3840	0	GLY		100 42.20 101 40.35	3 82.237	21.5		400.40
	. 3841	N	GLN GLN		101 41.00	yg 81.129	20.1 20.1		
	3842	CA CB			101 39.98			346 1.00	190.16
	3843 3844		GLN	В	101 39.25			370 1.00	
	70 3845			В	101 40.22	20. 10.014			
	, , , , , , , ,	,			·-				

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	3846 3847	OE1 NE2	GLN B	101 101	40.792 40.441 41.952	77.	845 565 596	23.140 22.378 19.731	1.00 1.00 1.00	190.16 190.16 128.49
	3848	C.		101 101	42.038	82.	780	19.407	1.00 1.00	128.49 164.10
	3849	O N	PRO B	102	42.675		.637 .258	19.115 19.540	1.00	192.64
	3850 3851	CD	PRO B	102	42.886 43.581		.010	18.018	1.00	164.10 192.64
	3852	CA	PRO B PRO B	102 102	44.669	79	.950	18.152 18.490	1.00 1.00	192.64
	3853	CB CB	PRO B	102	43.863		.733 .983	16.652	1.00	164.10
10	3854 3855	С	PRO B	102	42.928 42.017	80).208	16.389	1.00	164.10 147.70
10	3856	0	PRO B LEU B	102 103	43.418		.831	15.761 14.425	1.00 1.00	147.70
	3857	N CA	LEU B	103	42.870		1.913 3.136	14.328	1.00	111.28
	3858 3859	CB	LEU B	103 103	41.981 41.244	-	3.102	13.004	1.00	111.28 111.28
15	3860	CG	LEU B LEU B	103	40.261	. 8	1.951	13.100 12.716	1.00 1.00	111.28
	3861	CD1 CD2	LEU B	103	40.546	_	4.415 1.997	13.331	1.00	147.70
	3862 3863	С	LEU B	103 103	43.939 44.797	, 8	2.868	13.379	1.00 1.00	147.70 122.26
	3864	0	LEU B PHE B	104	43.890) 8	11.112	12.339 11.261	1.00	122.26
20	3865	N CA	PHE B	104	44.880	٠ .	31.157 79.951	11.311	1.00	249.69
	3866 3867	CB	PHE B	104 104	45.820 46.50	٠.	79.766	12.627	1.00 1.00	249.69 249.69
	3868	CG	PHE B PHE B	104	45.81	6	79.216	13.707 12. 79 3	1.00	249.69
0.5	3869	CD1 CD2	PHE B	104		٠.	80.137 79.041	14.939	1.00	249.69
25	3870 3871	CE1	PHE B	104			79.967	14.020	1.00	249.69 249.69
	3872	CE2	PHE B	104 104		73	79.416	15.096	1.00 1.00	122.26
	3873	CZ C	PHE B	104	44.22	27	81.185	9.885 9.546	1.00	122.26
20	3874 3875	ŏ	PHE B	104			80.290 82.207	9.093	1.00	122.11 122.11
30	3876	N	LEU B	10! 10!			82.309	7.743	1.00 1.00	103.82
	3877	CA	LEU B	10			83.676	7.495 8.466	1.00	103.82
	3878	CB	LEU B	10		70 .	84.000 85.309	8.040	1.00	103.82
35	3879 3880	CD1	LEU B	10 10			82.847	8.512	1.00	103.82 122.11
55	3881	CD2	LEU B	10			82.083	6.776 7.065	1.00 1.00	122.11
	3882	CO	LEU B	10	5 46.2		82.387 81.560	5.608	1.00	131.12
	3883 3884	Ň	ARG B	10			81.289	4.645		131.12 175.38
40		CA	ARG B		06 45.1 06 46.2	287	79.828	4.792 3.874		175.38
	3886	CB CG	ARG B	1	06 47.	384	79.387 77.897	3.980	1.00	175.38
	3887 3888	CD	ARG B			593 544	77.460	2.972	2 1.00	175.38 175.38
	3889	NE	ARG B			.536	76.259	2.40- 2.74		175.38
4:	5 3890	CZ NH1	ARG B		06 47	.618	75.361 75.963	1.47		175.38
	3891 3892	NH2	ARG B	1		.438 .418	81.578	3.22	0 1.00	131.12 131.12
	3893	C	ARG B			.374	81.096	2.78		139.30
_	3894	0	ARG L		107 46	3.184	82,394	2.50 1.12		139.30
5	3895 3896	N CA	CYS E	3		5.852	82.704 81.564	0.37	78 1.00	139.30
	3897	С	CYS S			6.515 7.7 4 7	81.560	0.2		139.30 152.04
	3898	0	CYS I	B	107 4	6.472	84.034	0.69 -0.8	78 1.00	152.04
	3899 55 3900	CB SG	CYS		107 +	J.853	84.704 80.604	-0.0	73 1.00	
•	55 3900 3901	И	HIS	В		5.703 6.205	79.419	-0.7		
	3902	CA		B. B.		5.429	78.180	-0.3 -0.7		137.70
	3903	CB CG		В	108 4	6.047	76.880 75.802	-1.3	1.00	137.70
	3904 60 3905		2 HIS	В		15.514 47.366	76.564	-0.4	1.00	
	3906	ND'		B B		47.609	75.341		919 1.00 453 1.00	40770
	3907			В	108	46.506	74.854 79.487		453 1.00 289 1.00	155.54
	3908 3909	· _	HIS	В	. • •	46.182 45.137	79.487 79. 7 31	-2.	900 1.0	
	65 3910	Ó	HIS	В		45.137 47.351	79.253		881 1.0 321 1.0	
	391	1 N	GLY GLY	8	109	47.480	79.271		.321 1.0 .866 1.0	0 164.07
	391		GLY	В	109	47.090	77.915 76.949		.098 1.0	0 164.07
	391 391	~	GLY	В	109 110	46.967 46.886 .	000	-6	.180 1.0	00 153.07
	70 391		TRP		0					

	C	ĊA	TRP B	110	46.506	76.568	-6.812 -8.097	1.00 1.00	153.07 171.40
	3916 3917	CB	TRP B	110	45.719	76.839 75.611	-8.920	1.00	171.40
	3917 3918	ÇG :	TRP B	110	45.467	74.833	-8.973	1.00	171.40
	3919	CD2	TRP B	110	44.256	73.764	-9.855	1.00	171.40
	3920	CE2	TRP B	110	44.496 42.998	74.937	-8.353	1.00	171.40
	3921	CE3	TRP B	110 110	46.040	75.000	-9.745	1.00	171.40
	3922	CD1	TRP B	110	45.778	73.889	-10.311	1.00	171.40 171.40
	3923	NE1 CZ2	TRP B	110	43.521	72.799	-10.140 -8.639	1.00 1.00	171.40
10	3924	CZ3	TRP B	110	42.026	73.974	-9. 52 6	1.00	171.40
10	3925 3926	CH2	TRP B	110	42.297	72.921 75.723	-7.098	1.00	153.07
	3927	C	TRP B	110	47.743	76.257	-7.296	1.00	153.07
	3928	0	TRP B	110	48.833 47.567	74.404	-7.104	1.00	188.19
	3929	N	ARG B	111 111	48.671	73.481	-7.333	1.00	188.19 249.69
15	3930	CA	ARG B	111	49.124	73.522	-8.790	1.00 1.00	249.69
	3931	CB CG	ARG B	111	48.394	72.532	-9.682 -11.018	1.00	249.69
	3932	CD	ARG B	111	49.101	72.359 70.961	-11.448	1.00	249.69
	3933 3934	NE	ARG B	111	49.00	69,965	-10.751	1.00	249.69
20	3935	CZ	ARG B	111	49.641 50.241	70.210	-9.587	1.00	249.69
LU	3936	NH1	ARG B	111	49.594	68.722	-11.216	1.00	249.69
	3937	NH2	ARG B ARG B	111	49.845	73.814	-6.431	1.00	188.19 188.19
	3938	C	ARG B	111	50.999	73.588	-6.787	1.00 1.00	160.66
25	3939	0 N	ASN B	112	49.534	74.350	-5.260 -4.291	1.00	160.66
25	3940	CA	ASN B	112		74.729	-3.648	1.00	209.47
	3941 3942	CB	ASN B	112		73.478 73.791	-2.372	1.00	209.47
	3943	CG	ASN B	112		74.947	-2.083	1.00	209.47
	3944	OD1	ASN B	112 112		72.757	-1.607	1.00	209.47
30	3945	ND2	ASN B ASN B	112		75.583	-4.931	1.00	160.66 160.66
	3946	C	ASN B ASN B	112		75.522	-4,489 -5,966	1.00 1.00	180.98
	3947	O N	TRP B	113	51.319	76.368	-6.608	1.00	180.98
	3948 3949	CA	TRP B	113		77.223 77.888	-7.8 63	1.00	248.40
35	3950	СВ	TRP B	113		77.037	-9.064	1.00	248.40
55	3951	CG	TRP B	113		77.029	-10.131	1.00	248.40
	3952	CD2	TRP B	113 113		76.102	-11.092	1.00	248.40 248.40
	3953	CE2	TRP B	11		77.717	-10.370	1.00 1.00	248.40
40	3954	CE3 CD1	TRP B	11		76.145	-9.405 -10.623	1.00	248.40
40	3955 3956	NE1	TRP B	11		75. 582 75.845	-12.289	1.00	248.40
	3957	CZ2	TRP B	11		75.843 77.461	-11.557	1.00	248.40
	3958	CZ3	TRP B	11		76.530	-12.504	1.00	248.40
	3959	CH2	TRP B	11		78.311	-5.641	1.00	180.98 180.98
45		Ç	TRP B		3 52.414	78.261	-4.452 -6.144	1.00 1.00	240.61
	3961	0 N	ASP B		14 53.465	79.305	-5.14 4 -5. 29 2		240.61
	3962 3963	CA	ASP B		14 53.905	80.407 80.596	-5,390		249.69
	3964	СВ	ASP B		14 55.427 14 56.207	79,633	-4.489	1.00	249.69
50	3965	CG	ASP B			79.644	-3.260		249.69
	3966	OD1	ASP B ASP B		14 55.981 14 57.054	78.868	-5.007		249.69 240.61
	3967	OD2	ASP B		14 53.185	81.707	-5.655		240.61
	3968	C	ASP B		14 53.064	82.062	-6.841 -4.627		153.55
5	3969 5 3970	Ň	VAL B		15 52.691		-4.82		153.55
٠,	3971	CA	VAL B		115 51.976		-4.13		146.14
	3972	СВ	VAL B		115 50.603 115 49.770		-4.64		146.14
	3973	CG1	VAL B		115 49.770 115 49.887		-4.38		146.14 153.55
	3974	CG2	VAL B		115 52.790	84.823	-4.25		153.55
6	0 3975	C	VAL		115 53.410	84.708	-3.19 -4.97		165.97
	3976	N	TYR	-	116 52.78		-4.57		165.97
	3977 3978	CA	TYR E	•	116 53.51		-5.61	-	249.69
	3979	CB	TYR	3	116 54.59		-5.72	22 1.00	249.69
(65 3980	CG	TYR		116 55.66 116 55.61		-6.71		249.69 249.69
	3981	CD1			116 56.58	2 84.386	-6.70		249.69 249.69
	3982	CE1 CD2		B	116 56.70	0 86.319	-4.86 -4.8		249.69
	3983	CE2		В	116 57.67		-4.89 -5.8		249.69
	3984 70 3985	CZ	TYR	В	116 57.61	11 84.360	-5.0		
	, 5 5555				•				

	986 987	OH C	TYR B	116	58.575 52.593 51.423	88. 88.	375 ,332 ,278	-5.898 -4.405 -4.782 -3.840	1.00 1.00 1.00 1.00	249.69 165.97 165.97 123.89
	988	0	TYR B	117	53.129		.413	-3.609	1.00	123.89
	989	N CA	LYS B	117	52.369 52.154		.641 .413	-4.924	1.00	248.40 248.40
	990 1991	CB	LYS B	117 117	53.310	92	323	-5.333 -6.340	1.00 1.00	248.40
3	1992	CG	LYS B	117	52.850	93	3.384	-5.761	1.00	248.40
	3993	CD CE	LYS B	117	51.729		1.253 5.311	-6.687	1.00	248.40 123.89
	3994 3995	NZ	LYS B	117	51.232 51.019		0.378	-2.948	1.00 1.00	123.89
	3996	С	LYS B	117 117	49.972	90	0.844	-3.40 9 -1.846	1.00	126.95
	3997	0	VAL B	118	51.055	; 8	9.650 9.314	-1.142	1.00	126.95
	3998	N CA	VAL B	118	49.843	,	7.999	-0.408	1.00	114.58 114.58
	3999 4000	СВ	VAL B	118 118	50.033 49.07	,	7.892	0.760	1.00 1.00	114.58
13	4001	CG1	VAL B VAL B	118	49.78	9 5	36.867	-1.372 -0.177	1.00	126.95
	4002	CG2 C	VAL B	118	49.29	•	90.352 91.007	0.547	1.00	126.95 120.13
	4003 4004	ŏ	VAL B	118	50.05 47.97	•	90.477	-0.179	1.00 1.00	120.13
20	4005	N	ILE B	119 119	47.24	4	91.402	0.686 -0.073	1.00	113.05
20	4006	CA	ILE B	119	46.81	13	92.633 93.628	0.860	1.00	113.05
	4007	CB CG2	ILE B	119	46.14 48.02	10	93.233	-0.750	1.00	113.05 113.05
	4008 4009	CG1	ILE B	119 119			94.049	-1.930 1.152	1.00 1.00	120.13
25	4010	CD1	ILE B	119			90.716	0.347	1.00	120.13
	4011	CO	ILE B	119	45.2		90.135 90.761	2.448	1.00	131.55 131.55
	4012 4013	N	. TYR B	120			90.162	2.952	1.00 1.00	143.62
	4014	CA	TYR B TYR B	120 120			89.457	4.286 4.186	1.00	143.62
30	4015	CB CB	TYR B TYR B	120	3 45.5		88.215 88.292	4,258	1.00	143.62
	4016	CD1	TYR B	12			87.153	4.175	1.00	143.62 143.62
	4017 4018	CE1	TYR B	12 12	•	966	86.963	4.019 3.930	1.00 1.00	143.62
	4019	CD2	TYR B		0 45.	733	85.821	4.010	1.00	143.62
35	4020	CE2 CZ	TYR B	12	0 47.	117	85.918 84.776	3.937	1.00	143.62 131.55
	4021 4022	он	TYR E	12	_	.898 .506	91.304	3.146		131.55
•	4023	C	TYR E			.919	92.426	3,396 3,013		134.10
	4024	O N	TYR	ā 1:	21 42	221	91.024 92.047	3.197	1.00	134.10 128.02
40	4025 4026	CA	TYR	_	- ·	,210),572	92.433	1.867		128.02
	4027	СВ	TYR			1.444	93.147	0.886 0.40		128.02
	4028	CG CD1			21 42	2.598	92.562 93.184	-0.61	2 1.00	128.02
AE	4029 4030	CE1	TYR	B 1		3.370 1.060	94.376	0.35	0 1.00	128.02 128.02
45	4031	CD2		_		1.810	95.003	-0.68 -1.14		
	4032	CE2	TYR TYR		121 4	2.970	94.395	-2.15	5 1.00	128.02
	4033	CZ OH	TYR	В	121 4	3.710	94.979 91.591	4.14	1.00	
5	4034 () 4035	Ċ.	TYR			10.085 39.556	90.483	4.0		124.90
ار.	4036	0	TYR LYS	8	122	39.716	92.457	5.0 6.0		124.90
	4037	N CA	LYS	В		38.635	92.165 92.121	7.4	42 1.0	
	4038 4039	22	LYS	В		39.152 38.059	91.814	8.4		404.00
5	5 4040	CG	LYS			38.511	92.092	9.8 10.8		0 161.09
	4041	CD		В	122	37.370	91.925 92.313	12.	1.0	0 161.09
	4042 4043		LYS	В	122	37.815 37.606	93.289		874 1.0 146 1.0	
	4044	C	LYS	В	122 122	37.892	94.448		146 1.0 437 1.0	00 160.91
(60 4045	, 0		8 B P B	123	36.409	92.939		250 1.0	00 160.91
	4048	•	AS AS	PΒ	123	35.338	93.908 94.474	6.	591 1.	00 179.88 00 179.88
	4047 4049	· ~	n AS	РΒ	123 123	34.877 34.061	93,486			00 179.88 00 179.88
	404	9 <u>C</u>		P B	123	33.105	92.913		.817 1. .583 1.	00 179.88
	65 405	~	ino AS	PB	123	34.365	93.289 95.056	4	.324	.00 160.91
	405 405	''	AS	SP B	123	35.719 35.556	96.222			.00 160.91
	405	3 () AS	SP B LY B	123 124	38.231	94.718			.00 138.47
	405	54	N G	LY B	124	36.604	95,728	•		
	70 40	,								

ar to

				404 2	7.853	96.561	2.426	1.00	138.47
	4056	С		124 3 124 3	7.655 8 <i>.2</i> 95	97.314	1.543	1.00	138.47
	4057	0			8.430	96.420	3.621	1.00	138.22
	4058	N .			9.627	97.168	4.009	1.00	138.22
_	4059	CA			9.534	97.532	5.496	1.00	228.57 228.57
5	4060	CB			8.461	98.543	5.849	1.00 1.00	228.57 228.57
	4061	CD CD	GLU B	125 3	8.835	99.938	5.425 5.952	1.00	228.57
	4062	OE1	GLU B			100.460	4.567	1.00	228.57
	4063 4064	OE2	GLU B		88.132	100.515 96.411	3.763	1.00	138.22
10	4065	C	GLU B		10.934	95.195	3.933	1.00	138.22
10	4066	0	GLU B		\$1.001	97.132	3.360	1.00	132.93
	4067	N	ALA B		41.974 43.266	96.495	3.155	1.00	132.93
	4068	CA	ALA B		44.225	97,478	2.531	1.00	135.56
	4069	CB	ALA B ALA B		43.730	96.115	4.563	1.00	132.93
15	4070	C	ALA B ALA B		43.549	96.898	5.489	1.00	132.93 121.91
	4071	0 N	LEU B		44.325	94.941	4.751	1.00 1.00	121.91
	4072	CA	LEU B	127	44.734	94.563	6.102 6.540	1.00	110.11
	4073 4074	CB	LEU B	127	43.939	93.352	8.046	1.00	110.11
20	4074 4075	CG	LEU B	127	43.777	93.371 94.684	8.464	1.00	110.11
20	4076	CD1	LEU B	127	43.167	92.200	8.476	1.00	110.11
	4077	CD2	LEU B	127	42.902 46.214	94.312	6.354	1.00	121.91
	4078	С	LEU B	127	46.818	94.960	7.211	1.00	121.91
	4079	0	LEU B	127 128	46.781	93.344	5.643	1.00	133.29
25	4080	N	LYS B LYS B	128	48.199	93.025	5.779	1.00	133.29
	4081	CA	LYS B LYS B	128	48.384	91.693	6.524	1.00	231.48 231.48
	4082	CB CG	LYS B	128	47.832	91.675	7.942	1.00 1.00	231.48
	4083	CD	LYS B	128	48.657	92.524	8.899 10.322	1.00	231.48
30	4084 4085	CE	LYS B	128	48.119	92.423	11.325	1.00	231.48
30	4086	NZ	LYS B	128	49.040	93.021 92.918	4.365	1.00	133.29
	4087	C	LYS B	128	48.770	92.760	3.392	1.00	133.29
	4088	0	LYS B	128	48.009 50.095	92.999	4.243	1.00	155.64
	4089	N	TYR B	129 129	50.722	92.894	2.930	1.00	155.64
35	4090	CA	TYR B	129	50.745	94.261	2.262	1.00	155.17 155.17
	4091	CB	TYR B	129	51.721	94.324	1.124	1.00 1.00	155.17
	4092	CG CD1	TYR B	129	51.372	93.892	-0.149 -1.184	1.00	155.17
	4093	CE1	TYR B	129	52.298	93.900	1.340	1.00	155.17
40	4094 4095	CD2	TYR B	129	53.026	94.765	0.315	1.00	155.17
40	4096	CE2	TYR B	129	53.965	94.775 94.340	-0.950	1.00	155.17
	4097	CZ	TYR B	129	53.593 54.521	94.360	-1.976	1.00	155.17
	4098	OH	TYR B	129	54.521 52.144	92.321	2.965	1.00	155.64
	4099	Ç	TYR B TYR B	129 129	52.930	92.644	3.857	1.00	155.64
45		0	TYR B	130	52.466	91.477	1.982	1.00	137.92 137.92
	4101	N	TRP B	130	53.792	90.873	1.883	1.00	181.18
	4102	CA CB	TRP B	130	53.871	89.553	2.659	1.00 1.00	181.18
	4103	CG	TRP B	130	53.301	89.553	4.048 5.275	1.00	181.18
50	4104 () 4105	CD2	TRP B	130	54.032	89.540	6.329	1.00	181.18
٦,	4106	CE2	TRP B	130	53.094	89.489 89.564	5.588		181.18
	4107	CE3	TRP B	130	55.398 51.980	89.516	4.397		181.18
	4108	CD1	TRP B	130		89.470	5.767		181.18
	4109	NE1	TRP B	130 130		89.458	7.667	1.00	181.18 181.18
5	5 4110	CZ2	TRP B	130		89.532	6.928		181.18
	4111	CZ3 CH2	TRP B	130		89.490	7.949		137.92
	4112	C	TRP B	130		90.577	0.427 -0.480		137.92
	4113 4114	ŏ	TRP B	130		90.655	0.220		207.31
e	50 4115	Ň	TYR B	131		90.218 89.871	-1.10		207.31
•	4116	CA	TYR B			90.207	-1.19		239.97
	4117	CB	TYR B			90.151	-2.60		239.97
	4118	CG	TYR B			91.130	-3.53		239.97
	4119	CD1	TYR B			91.065	-4.84		239.97
(65 4120	CE1	TYR B			89.101	-3.02		239.97 239.97
	4121	CD2 CE2				89.023	-4.32		239.97
	4122	CZ	TYR E	13		90.007	-5.23 -6.53		239.97
	4123 4124	OH	TYR E	3 13		89.922	-6.50 -1.20		207.31
	70 4125	C	TYR E		55.745	88.361	-1.20		
	, 0 4,20				•				

						87.903	-1.669	1.00	207.31
	4406	0		•	.000	87.590	-0.805	1.00	245.95
	4126 4127	Ň	GLU B 1		.760	86.133	-0.780	1.00	245.95
	4128	CA			3.632 7.906	85.470	-0.236	1.00	249.39
	4129	СВ).071	85.349	-1.220	1.00	249.39
5	4130	CG			2.448	83.901	-1.491	1.00	249.39 249.39
•	4131	CD			3.976	83.011	-0.751	1.00 1.00	249.39
	4132	OE1			0.223	83.649	-2.43B 0.271	1.00	245.95
	4133	OE2		132 5	5.535	86.097	1.341	1.00	245.95
	4134	CO	GLU B	132 5	5.697	86.700	0.003	1.00	176.11
10	4135	N	ASN B		4.430	85.403 85.462	0.965	1.00	176.11
	4136 4137	CA	ASN B		3.339	84.935	0.335	1.00	160.36
	4138	СВ	ASN B		2.010 51.822	B3.434	0.412	1.00	160.36 160.36
	4139	CG	ASN B		2.741	82.660	0.161	1.00	160.36
15	4140	OD1	ASN B		50.589	83.015	0.716	1.00 1.00	176.11
	4141	ND2	ASN B ASN B		53.555	84.965	2.388 2.802	1.00	176.11
	4142	C	ASN B	133	54.66 5	84.633	3.151	1.09	182.29
	4143	O N	HIS B		52.479	84.997	4.534	1.00	182.29
20	4144	CA	HIS B		52.525	84.611 85.860	5.391	1.00	249.69
20	4145 4146	CB	HIS B		52.743	85.559	6.845	1.00	249.69
	4147	CG .	. HIS B		53.003 52,286	85.883	7.951	1.00	249.69
	4148	CD2	HIS B	134	54.081	84.836	7.264	1.00	249.69 249.69
	4149	ND1	HIS B	134 134	54.036	84.709	8.595	1.00	249.69
25	4150	CE1	HIS B HIS B	134	52.961	85.335	9.023 4,873	1.00 1.00	182.29
	4151	NE2	HIS B	134	51.200	83.948	3.984	1.00	182.29
	4152	C O	HIS B	134	50.446	83.556	6.163	1.00	162.56
	4153	N	ASN B	135	50.922	83. 832 83.206	6.644	1.00	162.56
30	4154 4155	ĞA	ASN B	135	49.712	81.712	6.908	1.00	240.35
30	4156	CB	ASN B	135	49.964	80.928	5.625	1.00	240.35
	4157	CG	ASN B	135 135	50.213 49.484	81.111	4.647	1.00	240.35 240.35
	4158	OD1	ASN B	135	51.216	80.048	5.620	1.00 1.00	162.56
	4159	ND2	ASN B	135	49.252	83.905	7.919 9.028	1.00	162.56
35		C	ASN B	135	49.536	83.439	7.745	1.00	151.20
	4161	N	ILE B	136	48.544	85.024 85.840	8.846	1.00	151.20
	4162 4163	ČA	ILE B	136	47.996	86.737	8.329	1.00	153.45
	4164	CB	ILE B	136	46.845 45.775	85.891	7.675	1.00	153.45
40		CG2	ILE B	136	46.230	87.526	9.477	1.00	153.45 153.45
• •	4166	CG1	ILE B	136 136	45.072	88.386	9.042	1.00 1.00	151.20
	4167	CD1	ILE B	136	47.495	85.052	10.063 10.041	1.00	151.20
	4168	C O	!LE B	136	46.403	84.466	11.133		137.33
4	4169	Ň	SER B	137	48.291	85.084 84.351	12.353		137.33
4	5 4170 4171	CA	SER B	137	47.981	83.553	12.782	1.00	185.84
	4172	СВ	SER B	137	49.199 48.986	82.999	14.062		185.84
	4173	OG	SER B	137 137	47.481	85.154	13.549		137.33 137.33
	4174	Č	SER B	137	47.862	86.294	13.764		147.08
5	0 4175	0	ILE B	138	46.641	84.509	14.348 15.529	-	147.08
	4176	N GA	ILE B	138	46.043	85.114	15.24		140.24
	4177	CB	ILE B	138		85.533	16.54		140.24
	4178 4179	CG2	ILE B	138		85.830 86.736	14.30	7 1.00	140.24
4	55 4180	CG1	ILE B			87.030	13.73	7 1.00	140.24
•	4181	CD1	ILE B			84.165	16.72		147.08 147.08
	4182	C	ILE B			83.059	16.67		249.69
	4183	0	ILE B THA B			84.623	17.80		249.69
	4184	N	THR B			83.857	19.03 19.85		249.31
	60 4185	CA CB	THR B		9 47.944	84.369	20.00		249.31
	4186	OG1		3 13		85.783 84.099	19.12		249.31
	4187 4188	CG2	THR E	3 13		84.015	19.8	32 1.00	249.69
	4189	C	THR E	3 13		83.158	19.7	95 1.00	249.69 177.26
	65 4190	0	THR				20.5		
	4191	N	ASN I	_	10 44.211	85.439	21.3		040.00
	4192				0 44.612	86.358	22.5 23.3		249.69
	4193				40 43.435		23.8		040.00
	4194 70 4195			В 1	40 42.422	87.240	امكن		
	70 4195	, 32			•				

						aa ca4	24.665	1.00	249.69
	1196	ND2		140	43.566	86.631 86.161	20.396	1.00	177.26
	4197	С		140	43.247	87,200	19.812	1.00	177.26
	4198	o:	70	140	43.596	85.615	20.236	1.00	147.92
	4199	N .		141	42.040 41.050	86.199	19.327	1.00	147.92
	4200	CA	/\L.	141 141	40.337	85.085	18.551	1.00	170.82
	4201	СВ	,	141	40.015	87.128	19.967	1.00	147.92
	4202	C	ALA B ALA B	141	39.333	86.783	20.942	1.00	147.92 150.18
	4203	0	ALA B THR B	142	39.910	88.316	19.389	1.00 1.00	150.18
	4204	N CA	THR B	142	38.966	89.325	19.840 19.549	1.00	194.09
10	4205	CA CB	THR B	142	39.487	90.741	20.055	1.00	194.09
	4206	OG1	THR B	142	40.823	90.870	20.202	1.00	194.09
	4207 4208	CG2	THR B	142	38.595	91.777 89.119	19.053	1.00	150.18
	4209	C	THR B	142	37.681	88.485	17.996	1.00	150.18
15	4210	0	THR B	142	37.682 36.580	89.650	19.560	1.00	151.70
13	4211	N	VAL B	143	35.325	89.489	18.859	1.00	151.70
	4212	CA	VAL B	143 143	34.128	89.829	19.752	1.00	138.48 138.48
	4213	CB	VAL B	143	34.053	91.341	19.973	1.00	138.48
	4214	CG1	VAL B	143	32.853	89.308	19.122	1.00 1.00	151.70
20	4215	CG2	VAL B	143	35.313	90.418	17.658 16.688	1.00	151.70
	4216	C	VAL B	143	34.595	90.168	17,716	1.00	158.91
	4217	Ň	GLU B	144	36.106	91.488 92.427	16.609	1.00	158.91
	4218 4219	CA	GLU B	144	36.149	93.708	16.996	1.00	246.81
25	4220	CB	GLU B	144	36.870	94.445	18.127	1.00	246.81
23	4221	CG	GLU B	144	36.208 37.054	94.424	19.371	1.00	246.81
	4222	CD	GLU B	144	38.183	94.958	19.317	1.00	246.81
	4223	OE1	GLU B	144 144		93.872	20.396	1.00	246.81 158.91
	4224	OE2	GLU B GLU B	144		91.811	15.407	1.00 1.00	158.91
30	4225	C	GLU B	144		92.346	14.312	1.00	116.08
	4226	0 N	ASP B	145	37.485	90.676	15.606 14.501	1.00	116.08
	4227	CA	ASP B	145		89.992	15.039	1.00	169.83
	422B 4229	CB	ASP B	145		88.943 89.560	15.570	1.00	169.83
35	4230	CG	ASP B	145		90,286	14.797	1.00	169.83
33	4231	OD1	ASP B	145		89.327	16.756	1.00	169.83
	4232	OD2	ASP B	145 145		89.332	13.575	1.00	116.08 116.08
	4233	С	ASP B	14		88.992	12.450	1.00	118.95
	4234	0	ASP B SER B	14		89.161	14.054	1.00 1.00	118.95
40	4235	N	SER B	14		88.538	13.267	1.00	193.19
	4236	CA CB	SER B	14	6 33.592		14.116 15.261	1.00	193.19
	4237 4238	OG	SER B	14	6 33.830		12.048		118.95
	4239	č	SER B	14			12.186		118.95
45	4240	Ö	SER B	14			10.863	1.00	175.20
43	4241	N	GLY B	14			9.668	1.00	175.20
	4242	CA	GLY B	14	47 34.22		8.406		175.20 175.20
	4243	Ç	GLY B		47 34.16	2 87.487	8.467		119.45
	4244	0	THR B		48 34.35	0 89.383	7.260		119.45
50) 4245	N CA	THR B		48 34.44		5.967 5.057		97.36
	4246	ČB	THR B	1	48 33.22		4.118		97.36
	424 <i>1</i> 4248	OG1	THR B		48 33.60		5.90		97.36
	4249	CG2	THR B		48 32.06		5.25		119.45
5:	5 4250	С	THR B		48 35.80 48 36.10		4.83		119.45
	4251	0	THR B		48 36.10 49 36.61		5.13		115.49 115.49
	4252	N	TYR B		49 37.9		4.52		121.92
	4253	CA	TYR B		49 38.9	66 87.3 5 0	5.38		121.92
_	4254	CB CG	TYR B		149 39.0	73 87.793	6.83		121.92
0	0 4255	CD1	TYR B		149 38.1		7.77 9.10		121.92
	4256 4257	CE1	TYR E	3	149 38.2		7.20		121.92
	4257 4258	CD2	TYR E	3	149 40:1		8.5	78 1.00	121.92
	4259	CE2	TYR E	3	149 40.2		9.4	96 1.00	121.92
•	55 4260	CZ	TYR	3	149 39.3 149 39.5		40.0	21 1.00	121.92
•	4261	OH	TYR E	5	149 39.5 149 38.0	400	3.1		115.49 115.49
	4262	C	TYR I		149 37.	182 86.708	2.6		105.13
	4263	0	TYR		150 39.0	ngs 87.895	2.4		105.13
	4264		TYR			437 87.467	1.0	1.00	
	70 4265		• • • •						

							0.005	1.00	148.24
	4000	СВ		150	38.454	88.037 89.480	-0.407	1.00	148.24
	4266 4267	ČĞ	TYR B	150	38.643	89.864	-1.214	1.00	148.24
	4268	CD1.		150	39.713 39.871	91.204	-1.645	1.00	148.24
	4269	CE1		150 150	37.724	90.461	-0.031	1.00 1.00	148.24 148.24
	4270	CD2		150	37.867	91.803	-0.454 -1.268	1.00	148.24
	4271	CE2 CZ	TYR B	150	38.946	92.168	-1.715	1.00	148.24
	4272	OH	TYR B	150	39.096	93.473 88.014	0.809	1.00	105.13
	4273 4274	Ċ.	TYR B	150	40.836	89.015	1.414	1.00	105.13
10	4275	0	TYR B	150 151	41.228 41.612	87.372	-0.057	1.00	132.14 132.14
10	4276	N	CYS B	151	42.986	87.840	-0.332	1.00 1.00	132.14
	4277	CA	CYS B	151	43.242	88.046	-1.822 -2.671	1.00	132.14
	4278	C O	CYS B	151	42.511	87.547 86.847	0.236	1.00	149.67
15	4279 4280	СВ	CYS B	151	44.018	85.150	-0.462	1.00	149.67
13	4280	SG	CYS B	151	43.926 44.288	88.798	-2.129	1.00	118.50
	4282	N	THR B	152 152	44.661	89.083	✓ •3.516	1.00	118.50 151.99
	4283	CA	THR B THR B	152	44.403	90.547	-3.887	1.00 1.00	151.99
	4284	CB OG1	THR B	152	45.395	91.385	-3.266 -3.430	1.00	151.99
20	4285	CG2	THR B	152	43.014	90.976	-3.689	1.00	118.50
	4286 4287	C	THR B	152	46.154	88.854 89.115	-2.768	1.00	118.50
	4288	Ö	THR B	152	46.951 46.544	88.378	-4.864	1.00	134.78
	4289	N	GLY B	153 153	47.956	88.132	-5.089	1.00	134.78 134.78
25	4290	CA	GLY B	153	48.309	87.906	-6.545	1.00 1.00	134.78
	4291	C	GLY B	153	47.419	87.747	-7.387 -6.842	1.00	183.95
	4292	0 N	LYS B	154	49.605	87.885 87.673	-8.199	1.00	183.95
	4293 4294	CA	LYS B	154	50.077	88.730	-8.542	1.00	202.68
30	4295	СВ	LYS B	154		88.679	-9. 971	1.00	202.68
50	4296	CG	LYS B	154 154		89.815	-10.237	1.00	202.68 202.68
	4297	CD	LYS B LYS B	154		89.756	-11.649	1.00 1.00	202.68
	4298	CE NZ	LYS B	154	54.131	90.860	-11.921 -8.377	1.00	183.95
25	4299	C	LYS B	154		86,268 85,900	-7.729	1.00	183.95
35	4300 4301	ŏ	LYS B	154		85.484	-9.253	1.00	214.72
	4302	N	VAL B	15! 15!		84.117	-9.558	1.00	214.72 178.34
	4303	CA	VAL B VAL B	15		83.155	-9.620	1.00 1.00	178.34
	4304	CB	VAL B	15		81.766	-10.018 -8.276		178.34
40	4305	CG1 CG2	VAL B	15		83.118 84.193	-10.931	1.00	214.72
	4306 4307	C	VAL B	15		84.738	-11.865		214.72
	4308	Ó	VAL B	15 15		83.636	-11.061		210.74 210.74
	4309	N	TRP B	15		83.695	-12.334		249.69
45		CA	TRP B		56 52.245	83.105	-13.514 -13.504		249.69
	4311	CB CG	TRP B	1	56 51.997	81.615 80.576	-13.670		249.69
	4312 4313	CD2	TRP B		56 52.972	79.346	-13.606		249.69
	4314	CE2	TRP B		56 52.277 56 54. 3 58		-13.86		249.69
50	0 4315	CE3	TRP B		56 50.790	80.988	-13.35		249.69 249.69
	4316	CD1	TRP B TRP B		56 50.950	79.628	-13.41 -13.72		249.69
	4317	NE1 CZ2	TRP B		56 52.925		-13.72		249.69
	4318 4319	CZ3	TRP B	. 1	56 55.00		-13.91		249.69
5	5 4320	CH2	TRP B		156 54.285	400	-12.59	5 1.00	210.74
,	4321	С	TRP B		156 53.24 156 54.16		-12.05		210.74 156.28
	4322	0	TRP B		157 52.35	5 85.739	-13.40		156.28
	4323	N CA	GLN E		157 52.40		-13.76 -15.07		249.69
	4324	CB	GLN E	3	157 53.20		-14.9		249.69
•	50 4325 4326	ČĞ	GLN E	3	157 54.71	20.074	-14.0	19 1.00	249.69
	4327	CD	GLN S	-	157 55.32 157 55.27	-0 400	-14.3		249.69
	4328	OE1			157 55.27 157 55.90	6 87.860	-12.8		249.69 156.28
	4329	NE2	GLN GLN		157 51.00	35 87.808	-13.8		
1	65 4330	CO	GLN		157 50.8	93 88.830	-14.5 -13.2		
	4331 4332	N	LEU	В	158 50.0		-13.2	267 1.00	204.79
	4332	CA	LEU	В	158 48.6 158 47.7		-14.1	156 1.00	
	4334	CB	LEU	B	158 47.7 158 47.8	07 470	-15.0	669 1.00	162.40
	70 4335	CG	LEU	_					

.•

							16 250	1.00	162.40
				158	46.441	87.082	-16.258		
	4336	CD1				88.518	-16.037	1.00	162.40
		CD2	LEU B	158	48.464			1.00	204.79
	4337	CDZ			48.124	87.959	-11.852		
	4338	C	LEU B	158			-10.964	1.00	204.79
			LEU B	158	48.450	87.172			211.13
	4339	0			47.277	88.961	-11. 64 8	1.00	
		N	ASP B	159			-10.351	1.00	211.13
	4340			159	46.66 9	89.179			203.85
	4341	CA	ASP D			90.659	-10.178	1.00	
		СВ	ASP B	159	46.316		-10.416	1.00	203.85
	4342			159	47.491	91.574		1.00	
	4343	CG	ASP B			91.461	-9.680	1.00	203.85
			ASP B	159	48.489			1.00	203.85
	4344	OD1			47.413	92.407	-11.342		
10	4345	OD2	ASP B	159			-10.208	1.00	211.13
10			ASP B	159	45.397	88.344		1.00	211.13
	4346	С	ASF D		44.695	88.096	-11.193		
		0	ASP B	159			-8.984	1.00	157.46
	4347		TYR B	160	45.101	87.907			157.46
	4348	N	ITH			87.12 9	-8.729	1.00	
		CA	TYR B	160	43.891		-8.836	1.00	182.37
	4349			160	44.174	85.638			182.37
15	4350	CB				85.232	-10.147	1.00	
13		CG	TYR B	160	44.781		-10.315	1.00	182.37
	· 4351			160	46.161	85.213			
	4352	CD1	TYR B			84.810	-11.517	1.00	182.37
		CE1	TYR B	160	46.733		-11.217	1.00	182.37
	4353		7.00	160	43.977	4.849ک			
	4354	CD2	TYR 6			84.446	-12.433	1.00	182.37
	4007		TYR B	160	44.537			1.00	182.37
20	4355	CE2		160	45.917	84,423	-12.578		
	4356	CZ	TYR B			83.987	-13.765	1.00	182.37
			TYR B	160	46.481	83.867		1.00	157.46
	4357	ОН			43.275	87.423	-7.372		
	4358	С	TYR B	160			-6.377	1.00	157.46
			TYR B	160	43.977	87.686			159.09
	4359	0	ITH			87.358	-7.357	1.00	
06		N	GLU B	161	41.947		-6.168	1.00	159.09
25	4360			161	41.161	87.625			
	4361	CA	GLU B			88.664	-6.527	1.00	208.73
		СВ	GLU B	161	40.085		-5.420	1.00	208.73
	4362		GLU -	161	39.125	89.081			
	4363	CG	GLU B			90.353	-5.769	1.00	208.73
			GLU B	161	38.358			1.00	208.73
	4364	CD			37,289	90.587	-5.169		
30	4365	OE1	GLU B	161		91.125	-6.633	1.00	208.73
30			GLU B	161	38.829			1.00	159.09
	4366	OE2	GLU D		40.553	86.311	-5.703		
	4367	С	GLU B	161		85.483	-6.531	1.00	159.09
			GLU B	161	40.167			1.00	135.59
	4368	0	GLO D		40.491	86.120	-4.386		
	4369	N	SER B	162			-3.798	1.00	135.59
			SER B	162	39.945	84.894			156.53
35	4370	CA	SER P			84.552	-2.508	1.00	
55		CB	SER B	162	40.698		-1,523	1.00	156.53
	4371		050 0	162	40.507	85.561			135.59
	4372	OG	SER B			85.022	-3.475	1.00	
			SER B	162	38.467			1.00	135.59
	4373	С	SEN D			86.125	-3.362		
	4374	0	SER B	162		83.891	-3.332	1.00	183.98
	43/4		GLU B	163	37.785			1.00	183.98
40	4375	N	GLU D			83.933	-2.974		
40	4070	CA	GLU B	163			-2.941	1.00	249.53
	4376		GLU B	163	3 35.794	82.514			249.53
	4377	CB	GLU B		-	81.880	-4.311	1.00	
		CG	GLU B	16	3 35.543		-5. 03 0	1.00	249.53
	4378		020	16		82.475			249.53
	4379	CD	GLU B			82.464	-4.456	1.00	
	7070	OE1	GLU B	16	3 33.229		-6.173	1.00	249.53
45	4380		020	16		82.945			183.98
-	4381	OE2	GLU B		•	84.544	-1.569	1.00	
			GLU B	16	3 36.369			1.00	183.98
	4382	С	GLU D			84,379	-0.818		
	4383	0	GLU B	16			-1,199	1.00	111.61
			PRO B	16	4 35.304	85. 2 73			194.84
	4384	N	FNO D			85.647	-2.030		
50) 4385	CD	PRO B	16			0.122	1.00	111.61
30	4300		PRO B	16	35.206	85.903	0.122		194.84
	4386	CA	PHO D			86.986	-0.090	1.00	
	4387	CB	PRO B	16	34.171		-1.015	1.00	194.84
		-		14	64 33.217	88.310			111.61
	4388	CG	PRO B			84,904	1.197	1.00	
		С	PRO B	- 10	64 34.778		0.926	3 1.00	111.61
	4389			4	64 33.994	83.997			125.70
5:	5 4390	0	PRO B			85.078	2.417	7 1.00	
J.	3 4000		LEU B	1	65 35.268		3.48		125.70
	4391	N				84.150			
	4392	CA	LEU B			83.241	3.77	1 1.00	110.19
			LEU B	1	65 36.104				110.19
	4393	CB				82.190	4.86		
	4394	CG	LEU B	1	65 35.906		4.80	5 1.00	110.19
_	400		LEU B		65 34.494	81.640			110.19
- 6	0 4395	CD1				81.076	4.71		
Ū		CD2	LEU B	1			4.77	5 1.00	125.70
	4396				65 34.468	84.800			125.70
	4397	С	LEU B			85.716	5.27		
		0	LEU B	, '	165 35.127		5.31		120.14
	4398				166 33.348	84.317			120.14
	4399	N	ASN E				6.57	7 1.00	
	CE 4400	CA	ASN E	3	166 32.809		6.63		189.75
C	55 4400		1011	-	166 31.283	84.695			189.75
\ <u>-</u>	4401	CB	ASN E				6.14	1.00	
		CG	ASN E	3	166 30.537				189.75
	4402				166 31.053	87.039	6.10		
	4403	OD1	ASN E				5.69	94 1.00	189.7
		ND2		В	166 29.300				120.14
	4404		. 7011	_			7.7	1.00	120.1
•	70 4405	С	ASN I	5	166 33.42				

						82,978	7.752	1.00	120.14
AA	106	0	ASN B	166	33.718 33.594	84.911	8.875	1.00	133.16
	107	N	ILE B	167 167	34.163	84.359	10.087	1.00	133.16 105.73
	108	CA:	ILE B	167	35.634	84.660	10.178	1.00	105.73
44	409	CB .	ILE B	167	36.159	84.179	11.513	1.00 1.00	105.73
	410	CG2	ILE B	167	36.355	83.972	9.038 9.039	1.00	105.73
	411	CG1 CD1	ILE B	167	37.820	84.256	11.319	1.00	133.16
	412	C	ILE B	167	33.510	84.926 86.140	11.480	1.00	133.16
	413 414	ŏ	ILE B	167	33.451	84.057	12.213	1.00	113.92
	415	N	THR B	168	33.058 32.409	84.557	13.402	1.00	113.92
	416	CA	THR B	168 168	30.931	84.189	13.377	1.00	138.53 138.53
	417	CB	THR B	168	30.347	84.678	12.163	1.00	138.53
4	14 18	OG1	THR B	168	30.214	84.810	14.563 14.728	1.00 1.00	113.92
	4419	CG2	THR B	168	33.018	84.135	15.019	1.00	113.92
	4420	C O	THR B	168	33.161		15.526	1.00	134.74
	4421	. N	VAL B	169	33.381		16.840	1.00	134.74
	4422 4423	CA	VAL B	169	33.953	705	17.049	1.00	119.12
	4424	CB	VAL B	169	35.207 35.482		18.518	1.00	119.12
	4425	CG1	VAL B	169 169	36.40	•	16.397	1.00	119.12 134.74
	4426	CG2	VAL B VAL B	169	32.86	4 85.249	17.868	1.00 1.00	134.74
	4427	C	VAL B VAL B	169	32.51	1 86.415	18.047 18.527	1.00	162.52
	4428	0 2	ILE B	170	32.32		19.532	1.00	162.52
05	4429	CA	ILE B	170	31.27		19.449	1.00	162.30
25	4430 4431	CB	ILE B	170	30.27		18.010	1.00	162.30
	4432	CG2	ILE B	170			19.881	1.00	162.30
	4433	CG1	ILE B	170			19.859	1.00	162.30 162.52
	4434	CD1	ILE B	170 170			20.932	1.00	162.52
. 30	4435	Ç	ILE B	170			21.122	1.00 1.00	183.47
:	4436	0	ILE B LYS B	171		14 84.869	· 21.923 23.278	1.00	183.47
	4437	N CA	LYS B	171		59 84.966	23.716	1.00	228.46
	4438	CB	LYS B	17			23.602	1.00	228.46
25	4439	CG	LYS B	17			23.398	1.00	228.46
35	4440 4441	CD	LYS B	17			24.538	1.00	228.46
	4442	CE	LYS B	17			24.377	1.00	228.46
	4443	NZ	LYS B	17 17		-4404	24.319	1.00	183.47 183.47
	4444	Ç	LYS B	17	-		25.525		249.69
40	4445	0	LYS B NAG B	22	·	145 62.916	-2.146 -2.430		249.69
	4446	C1 C2	NAG B	22	21 49.		-2.430 -2.707		249.69
	4447	N2	NAG B	2			-2.515		249.69
	4448 4449	C7	NAG B	2		,,,	-2.115	1.00	249.69
45	4450	07	NAG B			628 66.249 813 67.630	-2.819		249.69
45	4451	C8	NAG B			117 63.412	-3.61		249.69 249.69
	4452	cs	NAG B			258 64.240	-3.75		249.69
	4453	03	NAG B			.568 61.956	-3.44 -4.71	-	249.69
	4454	C4 O4	NAG B		21 51	.118 61.532	-3.06		249.69
50	4455	C5	NAG B	, 2		.362 61.063 6675 61.604	-1.91	2 1.00	249.69
	4456 4457	O5	NAG E	3			-2.69	8 1.00	249.69
	4458	C6	NAG E	3).751 59.637).700 59.612	-1.64		249.69
	4459	· O6	NAG E			1.927 60.395	-4.78		249.69 249.69
55	4460	C1	NAG E	-		3.144 60.683	-5.69		249.69
	4461	C2	NAG I NAG I			3. 93 2 61.775	-5.13		249.69
	4462	N2	NAG	_		5.211 61.597	-4.84 -4.9		249.69
	4463	C7 O7	NAG			5.800 60.524	4.0		249.69
۷۲	4464) 4465	Č8	NAG			5.954 62.796 2.654 61.043			249.69
60	4465 4466	C3	DAM	B				06 1.00	249.69
	4467	03	NAG			3.764 61.185 51.697 59.961	-7.6		249.69 249.69
	4468	C4	NAG		222	1.134 60.393	3.8-		0.40.00
	4469	04	DAN DAN	8		50 <i>-</i> 571 59.687			-40.00
6:	5 4470	C5	DAN DAN			51.140 59.32			- 10 00
	4471	O5 C6	NAG		222	49.642 58.55		979 1.00	249.69
	4472	06	NAG		222	48.276 58.93	_	289 1.00	220.33
	4473 4474	C1	NAG	В		27.093 65.37 27.619 64.79		606 1.00	
7	0 4475	C2	NAG	В	242	27.619 . 64.78	•		
,					•				

							4 0770	4.00	220.33
	4476	N2	NAG B	242	28.439	63.617	-1.372	1.00	
	4477	C7	NAG B	242	28.079	62.446	-1.890	1.00	220.33
		07	NAG B		27.061	62.304	-2.564	1.00	220.33
	4478	C8	NAG B		28.977	61,252	-1.616	1.00	220.33
_	4479		NAG B		28.417	65.869	-2.342	1.00	220.33
5	4480	င္က	NAG B		28.893	65.358	-3.579	1.00	220.33
	4481	03			27.524	67.092	-2.588	1.00	220.33
	4482	C4	NAG B		28.320	68.165	-3.127	1.00	220.33
	4483	04	NAG B			67.565	-1.278	1.00	220,33
	4484	C5	NAG B		26.849		-0.583	1.00	220.33
10	4485	O 5	NAG B	242	26.201	66.460	-1.552	1.00	220.33
10	4486	C6	NAG B	242	25.764	68.596		1.00	220.33
	4487	O6	NAG B	242	26.133	69.886	-1.090		
	4488	C1	NAG B	243	27.960	68.648	-4.371	1.00	233.97
	4489	C2	NAG B	243	28.552	70.043	-4.570	1.00	233.97
15		N2	NAG B	243	28.067	70.964	-3.561	1.00	233.97
13	4490	C7	NAG B	243	28.929	71.745	-2.911	1.00	233.97
	4491		NAG B	243	30.147	71.719	-3.114	1.00	233.97
	4492	07		243	28.358	72.696	-1.871	1.00	233.97
	4493	C8	NAG B		28.185	70.544	-5.960	1.00	233.97
	4494	cs	NAG B	243		71.840	-6.174	1.00	233.97
20	4495	O 3	NAG B	243	28.726	69.586	-6.984	1.00	233.97
	4496	C4	NAG B	243	28.751		-8.263	1.00	233.97
	4497	04	NAG B	243	28.443	70.118			233.97
	4498	C5	NAG B	243	28.175	68.165	·6.727	1.00	
	4499	O5	NAG B	243	28.488	67.756	-5.361	1.00	233.97
25	4500	Č6	NAG B	243	28.776	67.113	-7.637	1.00	233.97
23		06	NAG B	243	30.175	66.991	-7.430	1.00	233.97
	4501		MAN B	244	29.240	69.921	-9.345	1.00	229.91
	4502	C1	MAN B	244	28.260	69.705	-10.400	1.00	229.91
	4503	C2		244	27.196	70.659	-10.238	1.00	229.91
	4504	02	MAN B			69.691	-11.752	1.00	229.91
30	4505	C3	MAN B	,	28.001	69.355	-12.770	1.00	229.91
	4506	03	MAN B	244		70.989	-12.013	1.00	229.91
	4507	C4	MAN B	244	29.658	70.964	-13.307	1.00	229.91
	4508	04	MAN B	244	30.237		-10.933	1.00	229.91
	4509	C5	MAN B	244	30.732	71.128		1.00	229.91
35	4510	O 5	MAN B	244	30.062	71.170	-9.601		229.91
55	4511	C6	MAN B	244	31.699	72.322	-11.158	1.00	229,91
	4512	06	MAN B	244	31.180	73.559	-10.690	1.00	
		C1	NAG B	250	44.268	53.492	9.707	1.00	249.69
	4513	C2	NAG B	250	45.671	53.603	10.328	1.00	249.69
40	4514		NAG B	250	45.573	53.779	11.763	1.00	249.69
40	4515	N2	NAG B	250	45.937	52.792	12.578	1.00	249.69
	4516	C7		250	46.363	51.706	12.172	1.00	249.69
	4517	07	NAG B		45.811	53.044	14.074	1.00	249.69
	4518	C8	NAG B	250		54.790	9.702	1.00	249.69
	4519	, СЗ	NAG B	250	46.415	54.843	10.194	1.00	249.69
45	4520	03	NAG B	250	47.749	54.657	8.172	1.00	249.69
	4521	C4	NAG B	250	46.432		7,602	1.00	249.69
	4522	04	NAG B	250	47.008	55.826	7.640	1.00	249.69
	4523	C5	NAG B	250	44.994	54.460		1.00	249.69
	4524	O 5	NAG B	250	44,369	53.324	8.287		249.69
50	4525	C6	NAG B	250	44.929	54.206	6.139	1.00	
50	4526	0 6	NAG B	250	43.668	53.664	5.761	1.00	249.69
		C1	NAG B	274	23.582	59.809	24.027	1.00	249.69
	4527		NAG B	274	23,459	61.065	24.903	1.00	249.69
	4528	C2		274	24.613	61.181	25.777	1.00	249.69
	4529	N2	NAG B		24.999	62.374	26.223	1.00	249.69
55	4530	C7	NAG B	274		63.422	25.934	1.00	249.69
	4531	07	NAG B	274	24.418	62.415	27.133	1.00	249.69
	4532	C8	NAG B	274	26.218	60.997	25.741	1.00	249.69
	4533	CЗ	NAG B	274			26.451	1.00	249.69
	4534	Q3	NAG B	274		62.216	24.836	1.00	249.69
60	4535	C4	NAG B	274		60.745			249.69
50	4536	04	NAG B	274	19.788	60.553	25.637	1.00	249.69
	4537	C5	NAG B	274	21.198	59.506	23.958	1.00	249.69
		O5	NAG B	274		59.674	23.192	1.00	
	4538	C6	NAG B	274		59.255	22.962	1.00	249.69
-	4539	06	NAG B	274		58.209	22.054	1.00	249.69
65				335		78.660	5.286	1.00	249.69
	4541	C1	NAG B			77.658	6.389	1.00	249.69
	4542	C2	NAG B	335		78.372	7.651	1.00	249.69
	4543	N2	NAG B	335		78.063	8.668	1.00	249.69
	4544	C7	NAG B	335			8.611	1.00	249.69
70	0 4545	07	NAG B	335	5 49.823	77.166	0.011	1.00	2.5.00

						70 DEE	9.950	1.00	249.69
	45.40	C8			,,,,,,	78.865 76.938	6.115	1.00	249.69
	4548 4547	C3	10100			75.759	6.909	1.00	249.69
	4547 4548	03			2.790	76.553	4.647	1.00	249.69
	4549	C4 ·			2.852 4.131	75.970	4.410	1.00	249.69
5	4550	04			4.131 2.678	77.814	3.812	1.00	249.69
3	4551	C5	10.0		1.319	78.289	3.939	1.00	249.69
	4552	O5			2.935	77.564	2.334	1.00	249.69 249.69
	4553	C6			3.923	78.447	1.826	1.00	249.69
	4554	06			3.529	87.808	25.515	1.00 1.00	249.69
10	4555	C1			2.252	87.842	26.379 25.533	1.00	249.69
	4556	C2	NAG B		11.073	87.751	25.533 25.835	1.00	249.69
	4557	N2	NAG B	340 4	10.086	86.909	26.833	1.00	249.69
	4558	C7 O7	NAG B	340 4	40.099	86.177	24.882	1.00	249.69
15	4559	C8	NAG B	•	38.898	86.878	27.182	1.00	249.69
15	4560	C3	NAG B	•	42.235	89.153 89.172	28.061	1.00	249.69
	4561 4562	0 3	NAG B		41.117	89.304	27.991	1.00	249.69
	4563	C4	NAG B		43.537	90.587	28.606	1.00	249.69
	4564	O4	NAG B	•	43.566 44.768	89.134	27.069	1.00	249.69
20	4565	C5	NAG B	340 340	44.691	87.877	26.352	1.00	249.69 249.69
20	4566	O 5	NAG B	340	46.101	89.143	27.805	1.00	249.69
	4567	C6	NAG B	340	47.172	88.783	26.936	1.00	212.59
	4568	Q6	NAG B	366	28.566	86.792	5.084	1.00	212.59
	4569	C1	NAG B	366	2: .738	86.264	3.928	1.00 1.00	212.59
25	4570	C2	NAG B	366	28.623	85.657	2.952	1.00	212.59
	4571	N2	NAG B	366	28.903	84.360	3.019 3.883	1.00	212.59
	4572	C7 O7	NAG B	366	28.430	83.623	1.966	1.00	212.59
	4573	C8	NAG B	366	29.845	83.792	3.282	1.00	212.59
20	4574	cs	NAG B	366	26.966	87.413 86.895	2.319	1.00	212.59
30	4575 4576	03	NAG B	366	26.061	88.236	4,315	1.00	212.59
	4577	C4	NAG B	366	26.186	89.443	3.682	1.00	212.59
	4578	04	NAG B	366	25.698 27.096	88.607	5.499	1.00	212.59
	4579	C5	NAG B	366 366	27.723	87.423	6.036	1.00	212.59 212.59
35	4580	O 5	NAG B	366	26.361	89.288	6.648	1.00	212.59
-	4581	C6	NAG B NAG B	366	27.276	89.790	7.613	1.00 1.00	243.26
	4582	O6	NAG B	367	24.341	89.710	3.786	1.00	243.26
	4583	C1	NAG B	367	24.090	91.194	3.541	1.00	243.26
	4584	C2	NAG B	367	24.852	92.006	4.472 4.025	1.00	243.26
40	4585	N2 C7	NAG B	367	25.846	92.768	2.834	1.00	243.26
	4586	07	NAG B	367	26.167	92.827	5.058	1.00	243.26
	4587 4588	C8	NAG B	367	26.602	93.591 91.455	3.687	1.00	243.26
	4589	C3	NAG B	367	22.591	92.825	3,445	1.00	243.26
4:	5 4590	03	NAG B	367	22.313 21.820	90.586	2.689	1.00	243.26
т.	4591	C4	NAG B	367	20.423	90.749	2.897		243.26
	4592	04	NAG B	367 367	22.208	89.105	2.859		243.26 243.26
	4593	C5	NAG B	367		88.941	2.791		243.26
	4594	O 5	NAG B NAG B	367		88.219	1.777		243.26
5	0 4595	C6	NAG B	367		87.692	0.915 61.471		249.69
	4596	O6	LYS D	4	55.929	67.814	61.069		249.69
	4597	CB CG	LYS D	4	55.569	66.389	62.28		249.69
	4598	CD	LYS D	4	55.219	65.523	61.85		249.69
	4599 55 4600	CE	LYS D	4	54.831	64.103 63.215	63.02	-	249.69
-	4601	NZ	LYS D	4	54.503	68.782	59.37		226.67
	4602	C	LYS D		54.982	68.517	59.81	6 1.00	226.67
	4603	0	LYS D		53.862 58.551	70.102	60.76	6 1.00	226.67
	4604	N	LYS D		56.206	68.740	60.28		226.67 199.21
	60 4605	CA	LYS D		55.175	69.129	58.09		157.97
	4606	N	PRO D		56.399	69.692	57.50		199.21
	4607	CD	PRO D		54.056	69.192	57.15		157.97
	4608	CA	PRO D		54.551	70.184	56.10		157.97
	4609	CB	PRO E	_	56.009	69.877	56.0		400.04
	65 4610	CG	PRO		53.742	67.819	56.5 56.5		
	4611	C	PRO I		54.592		56.0		205.80
	4612		LYS	D 6			55.4		205.80
	4613 4614		LYS	D 6			56.4		
	70 4615			D 6	51.395) 65.500			
	70 4010	•			•				

					54 007	64.131	55.942	1.00	249.69
	4616	CG	LYS D	6	51.007 · 50.433	63.220	57.018	1.00	249.69
	4617	CD	LYS D	6		61.838	56.448	1.00	249.69
	4618	CE	LYS D	6	50.116	60.880	57.497	1.00	249.69
	4819	NZ	LYS D	6	49.665	66.599	54.246	1.00	205.80
5	4620	С	LYS D	6	51.263	67.075	54.362	1.00	205.80
	4621	0	LYS D	6	50.132	66.245	53.080	1.00	180.35
	4622	N	VAL D	7	51.797	· 66.425	51.823	1.00	180.35
	4623	CA	VAL D	7	51.082	66.148	50.636	1.00	112.97
	4624	CB	VAL D	7	52.002	66.692	49.350	1.00	112.97
10	4625	CG1	VAL D	7	51.369	66.752	50.884	1.00	112.97
	4626	CG2	VAL D	7	53.374	65.540	51.677	1.00	180.35
	4627	C	VAL D	7	49.846 49.935	64.315	51.772	1.00	180.35
	4628	0	VAL D	7	49.935 48.699	66.171	51.443	1,00	191.62
	4629	N	SER D	8	40.099 47.441	65.455	51.269	1.00	191.62
15	4630	CA	SER D	8	46.339	66.118	52.114	1.00	215.34
	4631	CB	SER D	8	46.315	67.528	51.940	1.00	215.34
	4632	OG.	SER D	8	47.066	65.475	49.790	1.00	191.62
	4633	C	SER D	8	47.587	66.285	49.026	1.00	191.62
	4634	0	SER D	8 9	46.175	64.579	49.374	1.00	183.49
20	4635	N	LEU D LEU D	9	45.753	64.552	47.973	1.00	183.49
	4636	CA	LEU D	9	46.289	63.316	47.250	1.00	153.82
	4637	CB	LEU D	9	47.793	63.054	47.150	1.00	153.82
	4638	CG		9	48.011	61.992	46.080	1.00	153.82
~~	4639	CD1	LEU D LEU D	9	48.557	64.312	46.800	1.00	153.82
25	4640	CD2	LEU D	9	44.243	64.561	47.836	1.00	183.49
	4641	Ç	LEU D	9	43.522	64.243	48.781	1.00	183.49
	4642	0	ASN D	10	43.769	64.929	46.650	1.00	161.08
	4643	N	ASN D	10	42.340	64.954	46.383	1.00	161.08
20	4644	CA CB	ASN D	10	41.701	66.192	46.999	1.00	220.60
30	4645	CG	ASN D	10	40.195	66.089	47.052	1.00	220.60
	4646	OD1	ASN D	10	39.645	65.222	47.732	1.00	220.60
	4647	ND2	ASN D	10	39.515	66.966	46.328	1.00	220.60
	4648 4649	C	ASN D	10	42.077	64.931	44.883	1.00	161.08
35	4650	ŏ	ASN D	10	42.376	65.903	44.187	1.00	161.08
33	4651	Ň	PRO D	11	41.505	63.830	44.368	1.00	193.66
	4652	CD	PRO D	11	41.212	63.723	42.927	1.00	148.22 193.66
	4653	CA	PRO D	11	41.077	62.602	45.052	1.00	148.22
	4654	СВ	PRO D	11	40.656	61.698	43.905	1.00	148.22
40	4655	ĊĠ	PRO D	11	40.146	62.658	42.901	1.00	193.66
40	4656	C	PRO D	11	42.161	61.959	45.924	1.00 1.00	193.66
	4657	Ö	PRO D	11	43.336	62.325	45.849 46.760	1.00	193.56
	4658	N	PRO D	12	41.772	60.982	46.769 47.062	1.00	138.53
	4659	CD	PRO D	12	40.402	60.544	47.644	1.00	193.56
45	4660	CA	PRO D	12	42.731	60.293 59.503	48.588	1.00	138.53
	4661	CB	PRO D	12	41.824		48.520	1.00	138.53
	4662	CG	PRO D	12	40.494	60.225 59.379	46.825	1.00	193.56
	4663	С	PRO D	12	43.633	59.096	47.204	1,00	193.56
	4664	0	PRO D	12	44.775	58.919	45.700	1.00	115.99
50	4665	N	TRP D	13	43.081	58.039	44.727	1.00	115.99
	4666	CA	TRP D	13	43.745 42.854	57.917	43.495	1.00	155.11
	4667	CB	TRP D	13	41.432	57.624	43.839	1.00	155.11
	4668	CG	TRP D	13	40.964	56.869	44.959	1.00	155.11
	4669	CD2	TRP D	13	39.560	56.822	44.873	1.00	155.11
55	4670	CE2	TRP D	13	41.596	56.233	46.022	1.00	155.11
	4671	CE3	TRP D	13	40.330	57.988	43.138	1.00	155.11
	4672	CD1	TRP D	13 13	39.192	57.509	43.751	1.00	155.11
	4673	NE1	TRP D	13	38.778	56.160	45.808	1.00	155.11
60	4674	CZ2	TRP D	13	40.824	55.569	46.957	1.00	155.11
60		CZ3	TRP D	13		55.538	46.844	1.00	155.11
	4876	CH2	TRP D	13		58.540	44.288	1.00	115.99
	4677	C	TRP D	13		59.565	43.618	1.00	115.99
	4678	0	ASN D	14		57.810	44.644	1.00	127.73
4 E	4679	N CA	ASN D	14		58.211	44.268	1.00	127.73
65		CB	ASN D	14		58.128	45.485	1.00	184.43
	4681 4682	ČG	ASN D	14		56.717	45.996	1.00	164.43
	4683	OD1	ASN D			56.039	46.369	1.00	164.43
	4684	ND2	ASN D			56.265	46.023	1.00	164.43
70	4685	C	ASN D			57.395	43.094	1.00	127.73
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						57.291	42.929	1.00	127.73
4	1686	0		14	49.361 47.202	56.825	42.304	1.00	124.12
	1687	N	ARG D	15	47.484	56.018	41.111	1.00	124.12
	4688	CA	ARG D ARG D	15 15	47.249	54.517	41.374	1.00	138.52
_ 4	4689	CB	ARG D	15	47.935	53.919	42.607	1.00	138.52 138.52
	4690	CG CD	ARG D	15	47.775	52.394	42.630	1.00 1.00	138.52
	4691	NE	ARG D	15	48.696	51.717	41.716 41.012	1.00	138.52
	4692 4693	CZ	ARG D	15	48.387	50.631	41.111	1.00	138.52
	4694	NH1	ARG D	15	47.175	50.091 50.084	40.211	1.00	138.52
	4695	NH2	ARG D	15	49.292	56.487	40.117	1.00	124.12
10	4696	С	ARG D	15	46.436 45.277	56.068	40.197	1.00	124.12
	4697	0	ARG D	15 16	46.825	57.344	39.182	1.00	134.05 134.05
	4698	N	ILE D	16	45.853	57.861	38.222	1.00	185.30
. ~	4699	CA CB	ILE D	16	45.666	59.359	38.405	1.00 1.00	185.30
15	4700	CG2	ILE D	16	44.824	59.635	39.645 38.464	1.00	185.30
	4701 4702	CG1	ILE D	16	47.047	60.016 61.514	38.379	1.00	185.30
	4703	CD1	ILE D	16	47.030	57.638	36.740	1.00	134.05
	4704	С	ILE D	16	46.150 47.301	57.474	36.330	1.00	134.05
20	4705	0	ILE D	16 17	45.088	57.650	35.944	1.00	221.22
	4706	N	PHE D PHE D	17	45.198	57.475	34.508	1.00	221.22 170.58
	4707	CA	PHE D PHE D	17	43.814	57.258	33.908	1.00	170.58
	4708	CB	PHE D	17	43.398	55.818	33.833	1.00 1.00	170.58
25	4709	CD1	PHE D	17	42.060	55.454	34.005 33.544	1.00	170.58
25	4710	CD2	PHE D	17	44.330	54.832	33,886	1.00	170.58
	4711 4712	CE1	PHE D	17	41.658	54.141 53.511	33.422	1.00	170.58
	4713	CE2	PHE D	17	43.932 42.590	53.167	33.594	1.00	170.58
	4714	CZ	PHE D	17	42.590 45.825	58.706	33.880	1.00	221.22
30	4715	Ç	PHE D	17 17	46.106	59.689	34.562	1.00	221.22 189.75
	4716	0	PHE D LYS D	18	46.023	58.646	32.569	1.00	189.75
	4717	N	LYS D	18	46.615	59.743	31.808	1.00 1.00	249.69
	4718	CA CB	LYS D	18	47.255	59.178	30.538 29. 66 3	1.00	249.69
25	4719	ca	LYS D	18	47.978	60.189	28.531	1.00	249.69
35	4720 4721	άΣ	LYS D	18	48.719	59.471 60.449	27.572	1.00	249.69
	4722	CE	LYS D	. 18	49.392	61.242	26.779	1.00	249.69
	4723	NZ	LYS D	18	48.405 45.573	60.806	31.450	1.00	189.75
	4724	C	LYS D LYS D	18 18	44.509	60.493	30.912	1.00	189.75 246.53
40	4725	0	LYS D GLY D	19	45.887	62.060	31.766	1.00 1.00	246.53
	4726	N CA	GLY D	19	44.979	63.151	31.467 32.607	1.00	246.53
	4727	Ç	GLY D	19		63.582	32.512	1.00	246.53
	4728 4729	ŏ	GLY D	19		64.620 62.794	33.680	1.00	150.48
45	4730	Ň	Grn D	20		63.103	34.849	1.00	150.48
73	4731	CA	GLU D	20		61.840	35.704		195.02
	4732	CB	GLU D	20 20		60.576	34.943		195.02 195.02
	4733	ÇG	GLU D	20		59.403	35.877		195.02
	4734	CD QE1	GLU D	20		59.054	36.735		195.02
50		OE2	GLU D	20	41.093	58.831	35.748 35.717		150.48
	4736 4737	c	GLU D	2	0 43.844	64.181	35.641		150.48
	4738	ŏ	GLU D	2		64.375 64.870	36.545		166.05
	4739	N	ASN D	2		65.916	37.407		168.05
55	5 4740	CA	ASN D	2		67.242	37.24		249.69
	4741	CB	ASN D	2	42.390	67.487	35.82		249.69 249.69
	4742	CG	ASN D	_	1 43.129	67.337	34.85		249.69
	4743	OD1	ASN D		1 41.130	67.891	35.72		166.05
-	4744	ND2 C	ASN D		21 43.632	65.566	38.90 39.41		166.05
6	() 4745 4746	ŏ	ASN D) 2	21 42.697	64.941 66.001	39.59		232.99
	4747	Ň	VAL [22 44.685	65,753	41.02		232.99
	4748	CA	VAL	-	22 44.836 22 45.811	64.598	41.27	1.00	144.01
	4749	CB	VAL. [_			40.94		144.01
6	5 4750	CG1	VAL I		22 47.232 22 45.711		42.7		144.01 232.99
	4751	CG2	VAL I		22 45.367	67.003	41.7		232.99
	4752	C	VAL		22 46.132	67.762	41.13	4	149.70
	4753 4754	Ň	THR		23 44.97		42.9 43.7		149.70
•	4754 70 4755	CA	THR		23 45.409	68.376	40. 7		
	, 5 7,55				•				

4789		4756	СВ	THR D	23 · 23	44.185 43.328	69.205 69.469	44.222 43.101	1.00 1.00 1.00	239.97 239.97 239.97
4788 C. THR D 23 45.802 68.833 45.130 1.00 149.70 5 4789 C. D. THR D 23 45.802 68.833 45.130 1.00 183.97 4781 N LEU D 24 48.291 68.833 45.130 1.00 183.97 4782 C. B. LEU D 24 48.291 68.833 45.130 1.00 183.97 4783 C. B. LEU D 24 48.291 68.813 68.117 45.847 1.00 149.27 4786 C. B. LEU D 24 49.182 68.623 44.535 1.00 149.27 4786 C. D. LEU D 24 49.182 68.623 44.315 1.00 149.27 4786 C. D. LEU D 24 48.292 69.583 47.247 1.00 149.27 4787 C. LEU D 24 48.292 69.583 47.247 1.00 149.27 4788 N LEU D 24 48.894 70.827 48.881 1.00 183.97 4788 N LEU D 24 48.894 69.414 48.891 1.00 183.97 4788 N LEU D 24 48.894 69.414 48.891 1.00 183.97 4789 N A THR D 25 47.842 69.414 48.891 1.00 183.97 4789 N C THR D 25 46.169 70.455 50.074 1.00 206.28 4770 CB THR D 25 46.169 70.455 50.074 1.00 206.28 4771 CB THR D 25 46.169 70.455 50.074 1.00 206.28 4773 CG2 THR D 25 46.169 70.455 50.0074 1.00 206.28 4774 C THR D 25 46.169 70.455 50.893 1.00 206.28 4775 O THR D 25 48.762 69.083 50.893 1.00 178.50 4776 N C YS D 26 49.723 71.137 51.109 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4776 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4777 C C C THR D 25 48.762 69.083 50.893 1.00 178.50 4778 C C THR D 25 48.762 69.083 50.893 1.00 178.50 4778 C C THR D 25 48.762 69.083 50.893 1.00 1.00 178.50 4778 C C THR D 25 48.762 69.083 50.893 1.00 1.00 178.50 4778 C C THR D 25 48.762 69.083 50.893 1.00 1.00 178.50 4778 C C C C C C C C C C C C C C C C C C						44.641				
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4821 CA PHE D 32 45.775 78.197 55.266 1.00 249.60 4823 CB PHE D 32 48.711 77.304 54.761 1.00 249.60 4824 CG PHE D 32 48.130 77.274 55.266 1.00 249.60 4824 CG PHE D 32 48.130 77.274 55.266 1.00 249.60 4824 CG PHE D 32 48.435 76.713 56.514 1.00 249.60	(55 4820					'8 77.888			249.69
4823 CB PHE D 32 46.711 77.304 4824 CG PHE D 32 48.130 77.274 55.266 1.00 249.6 4824 CG PHE D 32 48.435 76.713 56.514 1.00 249.6						32 45.77	78.197	~ 4 7		249.69
4824 CG PHE D 32 48.130 77.274 56.514 1.00 249.6				PHE	D					249.69
				PHE	D			-0.0		249.69
			CD.	1 PHE	D	JZ 40.4	».			

					10.404	77.800	54.494	1.00	249.69
	4826	CD2	PHE D	-	49.164	76.678	56.983	1.00	249.69
	4827	CE1	PHE D		49.752		54.954	1.00	249.69
		CE2	PHE D	32	50.487	77.770	56.198	1.00	249.69
	4828	cz	PHE D	32	50. <i>7</i> 79	77.207	55.325	1.00	249.69
_	4829	C	PHE D	32	46.086	79.681	54.671	1.00	249.69
5	4830	ŏ	PHE D	32	45.300	80.381		1.00	237.86
	4831		GLU D	33	47.241	80.150	55.802	1.00	237.86
	4832	N	GLU D	33	47.603	81.555	55.640		249.69
	4833	CA	GLU D	33	47.766	82.184	57.029	1.00	
	4834	CB		33	47.688	83.708	57.034	1.00	249.69
10	4835	CG	GLU D	33	46.478	84.238	56.256	1.00	249.69
	4836	CD	GLU D		45.351	83.734	56.476	1.00	249.69
	4837	OE1	GLU D	33	46.656	85.163	55.429	1.00	249.69
	4838	OE2	GLU D	33		81.908	54.779	1.00	237.86
	4839	С	GLU D	33	48.821	82.759	53.896	1.00	237.86
15	4840	Ö	GLU D	33	48.729	81.269	55.041	1.00	249.69
13	4841	Ñ	VAL D	34	49.957	81.553	54.302	1.00	249.69
		CA	VAL D	34	51.188	81.333	54.850	1.00	245.39
	4842	CB	VAL D	34	52.357	80.686	54.126	1.00	245.39
	4843	CG1	VAL D	34	53.648	81.015	56.343	1.00	245.39
	4844	CG2	VAL D	34	52.522	80.928		1.00	249.69
20	4845		VAL D	34	51.103	81.386	52.773	1.00	249.69
	4846	Ç	VAL D	34	50.330	80.567	52.254		249.69
	4847	0		35	51.900	82.188	52.065	1.00	249.69
	4848	N		35	51.963	82.160	50.603	1.00	
	4849	CA	SER D		51.850	83.577	50.033	1.00	241.64
25	4850	CB	SER D	35	53.028	84.324	50.300	1.00	241.64
20	4851	OG	SER D	35		81.559	50.188	1.00	249.69
	4852	С	SER D	35	53.307	81.400	48.997	1.00	249.69
	4853	Ō	SER D	35	53.587	81,243	51,184	1.00	249.69
	4854	Ň	SER D	36	54.137	80.654	50.953	1.00	249.69
20	4855	CA	SER D	36	55.455		51.841	1.00	249.69
30		СВ	SER D	38	56.516	81.325	53.201	1.00	249.69
	4856	OG.	SER D	36	56.379	80.950	51,227	1.00	249.69
	4857	C	SER D	36	55.430	79.150	52.354	1.00	249.69
	4858		SER D	36	55.650	78.692		1.00	216.36
	4859	0	THR D	37	55.147	78.389	50.176	1.00	216.36
35	4860	N	THR D	37	55.091	76. 944	50.267		218.49
	4861	CA		37	53.651	76.439	50.029	1.00	218.49
	4862	СВ		37	52.773	77.009	51.009	1.00	218.49
	4863	OG1	THR D	37	53.595	74,930	50.138	1.00	
	4864	CG2	THR D	-	56.027	76.399	49.193	1.00	216.36
40	4865	С	THR D	37		76.908	48.070	1.00	216.36
70	4866	0	THR D	37	56.067	75.372	49.539	1.00	249.68
	4867	N	LYS D	38	56.792	74.790	48.591	1.00	249.68
	4868	CA	LYS D	38	57.737	74.638	49.265	1.00	248.74
	4869	СВ	LYS D	38	59.115	75.962	49.786	1.00	248.74
45	4870	ÇG	LYS D	38	59.701		50.467	1.00	248.74
4)		CD	LYS D	38	61.060	75.782	50.933	1.00	248.74
	4871	CE	LYS D	38	61.627	77.123	51.599	1.00	248.74
	4872	NZ	LYS D	38	62.953	76.993	48.044	1.00	249.68
	4873		LYS D	38	57.259	73.445		1.00	249.68
	4874	C	LYS D	38	56.626	72.660	48.747	1.00	200.98
50		0	TRP D	39		73.197	46.775		200.98
	4876	N		39		71.944	46.137	1.00	193.49
	4877	CA	TRP D	39		72.188	45.096		193.49
	4878	CB	TRP D	39		72.634	45.638		
	4879	CG	TRP D			71.924	46.562		193.49
5:	5 4880	CD2	TRP D			72.649	46.669	1.00	193.49
J.	4881	CE2	TRP D			70.747	47.307	1.00	193.49
	4882	CE3	TRP D	39		73.727	45.247	1.00	193.49
	4883	CD1	TRP D	3		73.745	45.854		193.49
	4884	NE1	TRP D	3	9 52.822		47.487		193.49
6	0 4885	CZ2	TRP D) 3		72.242	48.124		193.49
U		CZ3	TRP C) 3	9 52.994	70.335	48.20		193.49
	4886	CH2	TRP C) 3	9 51.807	71.084	45.45		200.98
	4887		TRP (_	9 58.428	71.393			200.98
	4888	C	TRP		9 59.127	72.127	44.76		160.00
	4889	0	PHE		10 58.712	70.108	45.63	-	160.00
•	55 4890	N		_	10 59.896	~~ ~ 4 4	45.02		228.90
	4891	CA	PHE I	_	40 60.943	00.400	46.10		228.90
	4892	CB	PHE	_	40 61.397		46.93		
	4893	CG	PHE		40 60.620		47.99	9 1.00	228.90
	4894	CD1		_			46.67	77 1.00	228.90
•	70 4895	CD2	· PHE	ט י	40 62.611				

	4000	CE1	PHE D	40.	61.049	71.862	48.794	1.00	228.90
	4896	CE1 CE2	PHE D	40.	63.046	72.028	47.465	1.00	228.90
	4897 4898	CZ.	PHE D	40	62.263	72.477	48.526	1.00	228.90
	4899	c ·	PHE D	40	59.620	68.2 6 6	44.183	1.00	160.00
5	4900	ŏ	PHE D	40	59.908	67.142	44.615	1.00	160.00
3	4901	N	HIS D	41	59.088	68.469	42.976	1.00	161.00
	4902	CA	HIS D	41	58.786	67.371	42.052	1.00	161.00
	4903	CB	HIS D	41	58.044	67.915	40.844	1.00	195.26
	4904	、 CG	HIS D	41	57.679	66.868	39.847 38.493	1.00 1.00	195.26 195.26
10	4905	CD2	HIS D	41	5 7.6 80	66.881	40.216	1.00	195.26
	4906	ND1	HIS D	41	57.205	65.626 64.923	39.133	1.00	195.26
	4907	CE1	HIS D	41 41	56.928 57.207	65.660	38.073	1.00	195.26
	4908	NE2	HIS D HIS D	41	60.056	66.641	41.588	1.00	161.00
15	4909	C O	HIS D	41	60.798	67.153	40.751	1.00	161.00
13	4910	N	ASN D	42	60.280	65.437	42.118	1.00	193.10
	4911 4912	CA	ASN D	42	61.464	64.633	41.801	1.00	193.10
	4913	CB	ASN D	42	61.638	64.471	40.281	1.00	195.59
	4914	CG	ASN D	42	60.700	63.415	39.686	1.00	195.59
20	4915	OD1	ASN D	42	59.501	63.435	39.953	1.00	195.59 195.59
	4916	ND2	ASN D	42	61.240	62.506	38. 87 3 42. 3 97	1.00 - 1.00	193.10
	4917	C	ASN D	42	62.690	65.318 65.146	41.919	1.00	193.10
	4918	0	ASN D	42	63.810 62.462	66.092	43.456	1.00	217.79
0.5	4919	N	GLY D	43 43	63.540	66.809	44.120	1.00	217.79
25	4920	CA	GLY D GLY D	40 40	63.681	68.227	43.596	1.00	217.79
	4921	C	GLY D	43	63.883	69.166	44.372	1.00	217.79
	4922 4923	N	SER D	44	63.567	68.373	42.275	1.00	249.69
	4924	ĞA	SER D	44	63.675	69.669	41.598	1.00	249.69
30	4925	CB	SER D	44	63.508	69.497	40.083	1.00	225.92
30	4926	ÖĞ	SER D	44	64.485	68.631	39.546	1.00	225.92
	4927	С	SER D	44	62.620	70.652	42.085	1.00 1.00	249.69 249.69
	4928	0	SER D	44	61.423	70.374	41.997 42.579	1.00	241.20
	4929	N	LEU D	45	63.056	71.806 72.805	43.063	1.00	241.20
35	4930	CA	LEU D	45 45	62.110 62.841	74.084	43.488	1.00	237.73
	4931	CB	LEU D	45 45	61.948	75.186	44.070	1.00	237.73
	4932	CG CD1	LEU D	45	61.151	74.631	45.239	1.00	237.73
	4933 4934	CD2	LEU D	45	62.798	76.363	44.515	1.00	237.73
40	4935	C	LEU D	45	61.074	73.125	41.980	1.00	241.20
40	4936	ŏ	LEU D	45	61.365	73.051	40.783	1.00	241.20
	4937	N	SER D	46	59.865	73.470	42.416	1.00	233.99 233.99
	4938	CA	SER D	46	58.772	73.787	41.503 41.932	1.00 1.00	249.22
	4939	CB	SER D	46	57.494	73.050 73.250	40.995	1.00	249.22
45	4940	QG	SER D	46	56.444 58.506	75.285	41.441	1.00	233.99
	4941	C	SER D SER D	46 46	59.042	76.064	42.232	1.00	233.99
	4942	0 N	GLU D	47	57.648	75.671	40.502	1.00	249.69
	4943 4944	CA CA	GLU D	47	57.306	77.074	40.285	1.00	249.69
50	4945	CB	GLU D	47	57.093	77.311	38.786	1.00	249.69
50	4946	ČĠ	GLU D	47	58.330	77.026	37.945	1.00	249.69
	4947	CD	GLU D	47	58.089	77.248	36.471	1.00	249.69 249.69
	4948	OE1	GLU D	47	57.260	76.516	35.888 35.899	1.00 1.00	249.69
	4949	OE2	GLU D	47	58.728	78.156 77.618	41.063	1.00	249.69
55	4950	Ç	GLU D	47	56.102 55.889	78.827	41.111	1.00	249.69
	4951	0	GLU D	47 48	55.306	76.740	41.661	1.00	194.51
	4952	N CA	GLU D	48	54.159	77.204	42.424	1.00	194.51
	4953 495 4	CB	GLU D	48	53.081	76.117	42.492	1.00	249.69
60	4955	ČĠ	GLU D	48	51.885	76.488	43.366	1.00	249.69
50	4956	CD	GLU D	48	51.102	77.675	42.836	1.00	249.69
	4957	OE1	GLU D	48	50.401	77.515	41.814	1.00	249.69
	4958	OE2	GLU D	48	51.189	78.768	43.437	1.00 1.00	249.69 194.51
	4959	С	GLU D	48	54.611	77.576	43.826 44.311	1.00	194.51
65		0	GLU D	48	55. 64 5	77.100 78.438	44.472	1.00	208.13
	4961	N	THR D	49 49	53.834 54.134	78.889	45.831	1.00	208.13
	4962	CA	THR D	49	54.570	80.363	45.826	1.00	249.69
	4963 4964	CB OG1	THR D	49	53.575	81.153	45.159	1.00	249.69
70	4965	CG2	THR D	49	55.902	80.516	45.103	1.00	249.69
	.000					_			

	4966 4967	CO	THR D	49	52.905 53.022	78.729 78.579 78.765	46.737 47.958 46.127	1.00 1.00 1.00	208.13 208.13 217.97
	4968	N	ASN D	••	51.725 50.477	78.601	46.861	1.00	217.97
	4969	CA	ASN D		49.294	78.643	45.885	1.00	202.82
5	4970	CB	ASN D ASN D	50	47.963	78.742	46.592	1.00	202.82
	4971	CG OD1	ASN D	50	47.874	78.441	47.781	1.00 1.00	202.82 202.82
	4972	ND2	ASN D	50	46.924	79.156	45.865 47.545	1.00	217.97
	4973 4974	C	ASN D	50	50.539	77.236	47.072	1.00	217.97
10	4975	Ŏ	ASN D	50	51.219	76.338 77.071	48.653	1.00	198.36
10	4976	N	SER D	51	49.834 49.854	75.790	49.352	1.00	198.36
	4977	CA	SER D	51 51	49.201	75.920	50.738	1.00	249.69
	4978	CB	SER D SER D	51	47.794	76.051	50.640	1.00	249.69 198.36
1 =	4979	OG C	SER D	51	49.166	74.663	48.566	1.00 1.00	198.36
15	4980 4981	ŏ	SER D	51	49.350	73.484	48.876 47.555	1.00	249.63
	4982	Ň	SER D	52	48.375	75.019 74.019	46.739	1.00	249.63
	4983	CA	SER D	52	47.679 46.187	74.334	46.625	1.00	163.31
	4984	CB	SER D	52 52	45.563	74.298	47.891	1.00	163.31
20	4985	OG	SER D SER D	52	48.258	73.922	45.336	1.00	249.63 249.63
	4986	CO	SER D	52	48.011	74.780	44.489	1.00 1.00	249.63
	4987	N	LEU D	53	49.024	72.867	45.096 43.799	1.00	224.52
	4988 4989	CA	LEU D	53	49.637	72.642	43.989	1.00	138.37
25	4990	CB	LEU D	53	51.016	72.017 71.271	42.806	1.00	138.37
	4991	CG	LEU D	53	51.627 51.483	72.075	41.504	1.00	138.37
	4992	CD1	LEU D LEU D	53 53	53.089	70.983	43.128	1.00	138.37
	4993	CD2	LEU D	53	48.761	71.740	42.951	1.00	224.52 224.52
20	4994	C	LEU D	53	48.703	70.536	43.177	1.00 1.00	200.53
30	4995 4996	N	ASN D	54	48.080	72.325	41.973 41.115	1.00	200.53
	4997	CA	ASN D	54	47.219	71.538 72.402	40.513	1.00	228.73
	4998	СВ	ASN D	54	46.121 45.105	72.402	41.535	1.00	228.73
	4999	CG	ASN D ASN D	54 54	45.105 44.559	71.982	42.255	1.00	228.73
35	5000	OD1	ASN D ASN D	54	44.839	74.111	41.608	1.00	228.73 200.53
	5001	ND2 C	ASN D	54	47.977	70.834	40.003 39.639	1.00 1.00	200.53
	5002 5003	ŏ	ASN D	54	49.102	71.221	39.482	1.00	249.24
	5004	Ň	ILE D	55	47.341	69. 78 5 68.962	38.403	1.00	249.24
40	5005	CA	ILE D	55	47.874 48.369	67.589	38.934	1.00	185.84
	5006	CB	ILE D	55 55	48.373	66.564	37.819	1.00	185.84
	5007	CG2	ILE D	55	49.764	67.751	39.564	1.00	185.84 185.84
	5008	CG1 CD1	ILE D	55	50.346	66.474	40.129	1.00 1.00	249.24
45	5009 5010	Č.	ILE D	55	46.742	68.738	37.416 37.750	1.00	249.24
43	5011	ŏ	ILE D	55	45.735	68.117 69.251	36.205	1.00	249.05
	5012	N	VAL D	56	46.903 45.870	69.090	35.198	1.00	249.05
	5013	CA	VAL D VAL D	56 JS	45.719	70.362	34.349	1.00	249.53
	5014	CB	VAL D	56	44.353	70.370	33.664	1.00	249.53 249.53
50		CG1 CG2	VAL D	56	45.886	71.589	35.230	1.00 1.00	249.05
	5016 5017	C	VAL D	56	46.211	67.906	34.301 34.704	1.00	249.05
	5018	ŏ	VAL D	56	46.980	67.034 67.879	33.094	1.00	232.44
	5019	N	ASN D	57	45.641 45.859	66.786	32.143	1.00	232.44
5:	5 5020	CA	ASN D	57 57		67.311	30.708		224.76
	5021	CB	ASN D ASN D	57		67.743	30.292		224.76 224.76
	5022	CG OD1	ASN D	57	43.446	66.989	30.437		224.76
	5023 5024	ND2	ASN D	57	44.292	68.958	29.772 32.410		232.44
6		C	ASN D	57		66.031 66.398	31.940		232.44
U	5026	0	ASN D			64.963	33.186		180.25
	5027	N	ALA D			64.086	33.631		180.25
	5028	CA	ALA D ALA D			62.956	34.45		155.06 180.25
	5029	CB C	ALA D			63.508	32.55		180.25
Ć	55 5030 5031	ŏ	ALA D		8 48.587	62,620	31.79- 32.53		167.78
	5031	Ň	LYS C) 5		64.009	32.53 31.58		167.78
	5032	CA	LYS) 5			31.01	7 1.00	249.69
	5034	СВ	LYS				30.29		249.69
	70 5035	CG	LYS	, 5	J 31.110	;			

		CD	LYS D	59 ⁻	51.889	67.003	29.845	1.00	249.69 249.69
	5036	CE	LYS D	59	50.965	68.013	29.165	1.00 1.00	249.69
	5037 5038	NZ ·	LYS D	59	51.690	69.228	28.694 32.356	1.00	167.78
	5039	C	LYS D	59	52.159	62.654	33,500	1.00	167.78
5	5040	ŏ	LYS D	59	52.494	62.936 61.564	31.727	1.00	220.31
,	5041	N	PHE D	60	52.568	60.608	32.364	1.00	220.31
	5042	CA	PHE D	60	53 4	59.699	31.294	1.00	243.71
•	5043	СВ	PHE D	60	54.062 53.053	58.843	30.590	1.00	243.71
	5044	CG	PHE D	60 60	53.280	58.409	29.293	1.00	243.71
10	5045	CD1	PHE D PHE D	60	51.881	58.454	31.232	1.00	243.71
	5046	CD2	PHE D PHE D	60	52.357	57.600	28.639	1.00	243.71
	5047	CE1 CE2	PHE D	60	50.954	57.647	30.589	1.00 1.00	243.71 243.71
	5048	CZ	PHE D	60	51.194	57.217	29.287 33.202	1.00	220.31
15	5049 5050	c c	PHE D	60	54.571	61.240	34.207	1.00	220.31
13	5050	ŏ	PHE D	60	55.007	60.671 62.417	32.789	1.00	201.05
	5052	N	GLU D	61	55.025	63.125	33.487	1.00	201.05
	5053	CA	GLU D	61	56.101	64.332	32.653	1.00	249.69
	5054	CB	GLU D	61	56.5.°° 57.065	63.987	31.251	1.00	249.69
20	5055	ÇG	GLU D GLU D	61 61	56.045	63.244	30.385	1.00	249.69
	5056	CD	GLU D	61	54.897	63.728	30.245	1.00	249.69
	5057	OE1	GLU D	61	56.395	62.176	29.835	1.00	249.69 201.05
	5058	OE2 C	GLU D	61	55.671	63.588	34.884	1.00 1.00	201.05
25	5059	ŏ	GLU D	61	56.512	63.803	35.757	1.00	185.73
23	5060 5061	Ň	ASP D	62	54.359	63.735	35.086 36.371	1.00	185.73
	5062	CA	ASP D	62	53.815	64.165 64.502	36.245	1.00	180.28
	5063	CB	ASP D	62	52.334	65.480	35,132	1.00	180.28
	5064	CG	ASP D	62	52.063	66.360	34.882	1.00	180.28
30	5065	OD1	ASP D	62	52.924 50.985	65.379	34.514	1.00	180.28
	5066	OD2	ASP D ASP D	62 62	53.982	63.078	37.414	1.00	185.73
	5067	C	ASP D ASP D	62	53.979	63.353	38.606	1.00	185.73 159.27
	5068	0 N	SER D	63	54.106	61.837	36.960	1.00	159.27
35	5069	ČA	SER D	63	54.292	60.711	37.864 37.086	1.00 1.00	168.15
33	5070 5071	CB	SER D	63	54.380	59.390	36. 3 18	1.00	168.15
	5071	OG	SER D	63	53.226	59.160 60.949	38.595	1.00	159.27
	5073	Ċ	SER D	63	55.608	61.192	37.968	1.00	159.27
	5074	0	SER D	63	56.640 55.584	60.889	39.918	1.00	167.46
40	5075	N	GLY D	64 64	56.818	61.106	40.647	1.00	167.46
	5076	CA	GLY D	64	56.687	61.299	42.144	1.00	167.48
	5077	C	GLY D	64	55.643	61.035	42.741	1.00	167.46 249.05
	5078	0 N	GLU D	65	57.772	61.788	42.737	1.00 1.00	249.05
45	5079 5080	ĞA	GLU D	65	57.882	62.037	44.170 44.640	1.00	248.88
43	5081	CB	GLU D	65	59.223	61.476	46,061	1.00	248.88
	5082	CG	GLU D	65	59.604	61.791 61.571	46.298	1.00	248.88
	5083	CD	GLU D	65	61.083 61.892	62.265	45.646	1.00	248.88
	5084	OE1	GLU D	65 65	61.439	60.704	47.125	1.00	248.88
50	5085	OE2	GLU D	65 65	57.794	63.533	44.486	1.00	249.05
	5086	C	GLU D	65		64.318	43.989	1.00	249.05 212.16
	5087	0 N	TYR D	66	E0 000	63.924	45.319	1.00 1.00	212.16
	5088 5089	CA	TYR D	66	56.652	65.335	45.686 45.288	1.00	195.47
5:	5 5090	CB	TYR D	66		65.835	43.813	1.00	195.47
J.	5091	CG	TYR D	66		65.854 64.683	43.131	1.00	195.47
	5092	CD1	TYR D	66		64.715	41.795	1.00	195.47
	5093	CE1	TYR D	66		67.060	43.118	1.00	195.47
	5094	CD2	TYR D	66		67.105	41.789		195.47
6		CE2	TYR D			65.932	41.131		195.47
	5096	CZ	TYR D			65.982	39.822		195.47 212.16
	5097	OH C	TYR D			65.617	47.183		212.16
	5098	ŏ	TYR D		6 56.894	64.694	47.993		190.15
4	5099 5 5100	Ň	LYS D		7 56.848	66.906	47.534 48.92 0		190.15
U	5101	ČA	LYS) 6		67.355 68.895	49.512		181.22
	5102	СВ	LYS			66.886 67.251	48.66		181.22
	5103	CG	LYS				49.28	1.00	181.22
	5104	CD	LYS	-	7 60.788 7 61.948		48.28		181.22
7	70 5105	CE	LYS	, 6	. 01.010				

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	5106	NZ	LYS D	67 ·	63.216	66.167	40 074	4.00	404.00
	5107	C	LYS D	67	56.878	68.876	48.871 49.119	1.00 1.00	181.22
	5108	ŏ	LYS D	67	57.1 5 5	69.660	48.209	1.00	190.15 190.15
_	5109	N	CYS D	68	56.473	69.282	50.320	1.00	199.06
5	5110	CA	CYS D	68	56.346	70.695	50.654	1.00	199.06
	5111	C	CYS D	68	57.039	71.004	51.975	1.00	199.06
	5112	O _C D	CYS D	68	57.153	70.155	52.861	1.00	199.06
	5113 5114	CB SG	CYS D CYS D	68 68	54.871 53.830	71.135 70.461	50.708	1.00	219.86
10	5115	N	GLN D	69	57.505	72.240	52.050 52.083	1.00 1.00	219.86
	5116	CA	GLN D	69	58.212	72.728	53.257	1.00	249.17 249.17
	5117	CB	GLN D	69	59.714	72.495	53.072	1.00	249.69
	5118	CG	GLN D	69	60.606	73.364	53.942	1.00	249.69
15	5119	CD	GLN D	69	62.082	73.199	53.613	1.00	249.69
1.	5120 5121	OE1 NE2	GLN D GLN D	69 69	62.491	73.322	52.452	1.00	249.69
	5122	C	GLN D	69	62.892 57.925	72.925 74.222	54.634 53.407	1.00 1.00	249.69
	5123	ŏ	GLN D	69	57.726	74.927	52.418	1.00	249.17 249.17
	5124	N	HIS D	70	57.896	74.706	54.642	1.00	249.69
20	5125	CA	HIS D	70	57.642	76.122	54.874	1.00	249.69
	5126	CB	HIS D	70	56.693	76.309	56.060	1.00	249.61
	5127 5128	CG CD2	HIS D HIS D	70 70	55.290 54.464	75.881 75.035	55.773	1.00	249.61
	5129	ND1	HIS D	70	54.464 54.583	76.348	56.426 54.683	1.00 1.00	249.61
25	5130	CE1	HIS D	70	53.382	75.805	54.680	1.00	249.61 249.61
	5131	NE2	HIS D	70	53.280	75.003	55.727	1.00	249.61
	5132	Ç	HIS D	70	58.936	76.887	55.115	1.00	249.69
	5133	0	HIS D	70	60.031	76.352	54.920	1.00	249.69
30	5134 5135	N CA	GLN D GLN D	71	58.803	78.140	55.540	1.00	249.69
50	5136	CB	GLN D	71 71	59.955 59.459	79.008 80.374	55.802	1.00	249.69
	5137	CG	GLN D	71	60.461	81.539	56.307 56.197	1.00 1.00	249.69 249.69
	5138	CD	GLN D	71	60.863	81.861	54.754	1.00	249.69
25	5139	OE1	GLN D	71	60.016	81.976	53.858	1.00	249.69
35	5140	NE2	GLN D	71	62.163	82.021	54.530	1.00	249.69
	5141 5142	C	GLN D GLN D	71	60.929	78.392	56.816	1.00	249.69
	5143	N	GLN D	71 72	62.143 60.389	78.352 77.905	56.581 57.932	1.00	249.69
	5144	CA	GLN D	72	61.203	77.301	58.984	1.00 1.00	249.69 249.69
40	5145	СВ	GLN D	72	61.267	78.257	60.181	1.00	247.95
	5146	CG	GLN D	, 72	62.117	77.792	61.354	1.00	247.95
	5147	CD	GLN D	72	61.994	78.719	62.551	1.00	247.95
	5148 5149	OE1 NE2	GLN D GLN D	72 72	62.253	79.917	62.449	1.00	247.95
45	5150	C	GLN D	72	61.591 60.624	78.168 75.947	63.693 59.409	1.00 1.00	247.95
	5151	ŏ	GLN D	72	60.335	75.721	60.584	1.00	249.69 249.69
	5152	N	VAL D	73	60.449	75.052	58.443	1.00	248.81
	5153	CA	VAL D	73	59.911	73.726	58.720	1.00	248.81
50	5154 5155	CB CG1	VAL D	73	58.396	73.640	58.398	1.00	224.12
50	5158	CG2	VAL D VAL D	73 73	57.822 57.664	72.365	58.991	1.00	224.12
	5157	C	VAL D	73 73	60.641	74.863 72.704	58.936 57.858	1.00 1.00	224.12
	5158	ŏ	VAL D	73	60.991	72.985	56.717	1.00	248.81 248.81
	5159	N	ASN D	74	60.869	71.519	58.404	1.00	237.91
55	5160	CA	ASN D	74	61.552	70.475	57.660	1.00	237.91
	5161 5162	CB CG	ASN D	74	62.098	69.419	58.631	1.00	218.21
	5163	OD1	ASN D ASN D	74 74	63.003 63.818	70.022 70.893	59.699	1.00	218.21
	5164	ND2	ASN D	74	62.865	69.553	59.398 60.940	1.00 1.00	218.21
60	5165	С	ASN D	74	60.595	69.846	56.635	1.00	218.21 237.91
	5166	0	ASN D	74	59.477	69.450	56.973	1.00	237.91
	5167	N	GLU D	75	61.042	69.772	55.381	1.00	249.69
	5168 5169	CA	GLU D	75 75	60.252	69.219	54.276	1.00	249.69
65	5170	CB CG	GLU D	75 75	61.161 62.563	68.971 68.470	53.065	1.00	244.63
	5171	CD	GLU D	75 75	63.503	68.479 68.477	53.417 52.223	1.00 1.00	244.63
	5172	OE1	GLU D	75	63.579	69.508	51.523	1.00	244.63 244.63
	5173	OE2	GLU D	75	64.172	67.448	51.989	1.00	244.63
70	5174 5175	C	GLU D	75	59.463	67.954	54.609	1.00	249.69
70	5175	0	GLU D	75	59. 9 47	67.066	55.313	1.00	249.69

					ee 044	67.886	54,080	1.00	245.54
	5176	N		76 ·	58.244		54.313	1.00	245.54
		CA	SER D	76	57.338	66.759	53.739	1.00	192.35
	5177	CB		76	55.952	67.070		1.00	192.35
	5178	og.		76	55.961	66.977	52.328		245.54
_	5179		SER D	76	57.811	65.437	53.721	1.00	
	5180	C	SER D	76	58.617	65.413	52.791	1.00	245.54
	5181	0	GLU D	77	57.289	64.340	54.268	1.00	239.60
	5182	N	GLU D	77	57.628	63.013	53.788	1.00	239.60
	5183	CA	GLU D	77	56.972	61.938	54.663	1.00	249.69
	5184	CB	GLU D		57.497	61.895	56.089	1.00	249.69
10	5185	CG	GLU D	77		61.533	56.157	1.00	249.69
	5186	CD	GLU D	77	58.969	61.453	55.090	1.00	249.69
	5187	OE1	GLU D	77	59.621	61.333	57.282	1.00	249.69
	5188	OE2	GLU D	7 7	59.476	62.902	52.366	1.00	239.60
	5189	C	GLU D	77	57.106		52.139	1.00	239.60
15	5190	Ö	GLU D	7 7	55.898	62.905	51.386	1.00	190.36
13		Ň	PRO D	78	58.019	62.800	51.572	1.00	231.46
	5191	CD	PRO D	78	59.457	62.543		1.00	190.36
	5192	CA	PRO D	78	57.642	62.695	49.969	1.00	231.46
	5193	CB	PRO D	78	58.919	62.159	49.320		231.46
	5194	CG	PRO D	78	60.002	62.732	50.179	1.00	190.36
20	5195		PRO D	78	56.456	61.764	49.731	1.00	
	5196	C	PRO D	78	56.163	60.897	50. 55 3	1.00	190.36
	5197	. 0	VAL D	79	55.760	61.969	48.620	1.00	182.77
	5198	N		79	54.639	61.112	48.261	1.00	182.77
	5199	CA	VAL D		53.272	61.804	48.426	1.00	114.23
25	5200	CB	VAL D	79	52.173	60.961	47.770	1.00	114.23
	5201	CG1	VAL D	79		61.977	49.909	1.00	114.23
	5202	CG2	VAL D	79	52.957	60.799	46.800	1.00	182.77
	5203	С	VAL D	79	54.845	61.663	46.043	1.00	182.77
	5204	0	VAL D	79	55.292		46.397	1.00	172.05
30	5205	N	TYR D	80	54.538	59.570	45.004	1.00	172.05
50	5206	CA	TYR D	80	54.726	59.204	44.888	1.00	249.30
	5207	CB ·	TYR D	80	55.475	57.870	43.518	1.00	249.30
	5208	CG	TYR D	80	56.087	57.651		1.00	249.30
		CD1	TYR D	80	57.327	58.197	43.191	1.00	249.30
25	5209	CE1	TYR D	80	57.868	58.042	41.917	1.00	249.30
35	5210	CD2	TYR D	80	55.403	56.940	42.531		249.30
	5211	CE2	TYR D	80	55.937	56.780	41.254	1.00	249.30
	5212		TYR D	80	57.167	57.335	40.956	1.00	
	5213	CZ	TYR D	80	57.689	57.191	39.696	1.00	249.30
	5214	ÓН	TYR D	80	53.407	59.120	44.238	1.00	172.05
40	5215	Ç		80	52.419	58.550	44.701	1.00	172.05
	5216	0		81	53.407	59.702	43.054	1.00	138.80
	5217	N		81	52.239	59.681	42.207	. 1.00	138.80
	5218	CA	LEU D		51.837	61.099	41.821	1.00	163.84
	5219	СВ	LEU D	81	50.683	61.126	40.812	1.00	163.84
45	5220	CG	LEU D	81	49,462	60.512	41.463	1.00	163.84
	5221	CD1	LEU D	81		62.539	40.357	1.00	163.84
	5222	CD2	LEU D	81	50.394	58.907	40.932	1.00	138.80
	5223	С	LEU D	81	52.560	59.196	40.251	1.00	138.80
	5224	0	LEU D	81	53.554		40.598	1.00	140.95
50	5225	N	GLU D	82		57.924	39.380	1.00	140.95
50	5226	CA	GLU D	82		57.149	39.716		249.69
	5227	СВ	GLU D	82		55.662	38.685	1.00	249.69
	5228	ČĠ	GLU D	82		54.915			249.69
		CD	GLU D	82	53.177	53.447	39.028		249.69
<i>E</i> 6	5229	OE1	GLU D	82	53.282	53.118	40.233		249.69
55		OE2	GLU D	82	53.238	52.623	38.088	1.00	140.95
	5231		GLU D	82		57.324	38.415		140.95
	5232	C	GLU D	82		57.287	38.824		
	5233	0	VAL D	83		57. 53 3	37.139		204.94
_	5234	N	VAL D			57.704	36.106		204.94
6	0 5235	CA				58.985	35.282	2 1.00	154.41
	5236	CB	VAL D	_		59.119	34.24		154.41
	5237	CG1	VAL D			60.203	36.20	7 1.00	154.41
	5238	CG2	VAL D			56.510	35.15		204.94
	5239	С	VAL D			55.962	34.78		204.94
6	5 5240	0	VAL D		3 51.125		34.75		140.70
J	5241	N	PHE C	_	48.858	56.137	33.91		140.70
	5242	CA	PHE C		48,655	54.961	34.73		172.63
	5243	СВ	PHE C		34 48.013		35.90		172.63
	5244	CG	PHE E) (34 48.828		37.10		172.63
-	70 5245	CD1	PHE		34 48.823	54.095	37.10		,, 2.30
- 1	U 3243								

		000	PHE D	84	49.579	52.229	35.815	1.00	172.63
	5246	CD2 CE1			49.553	53.648	38.187	1.00	172.63
	5247	CE2	PHE D		50.310	51.776	36.892	1.00	172.63
	5248	CZ	PHE D		50.298	52.483	38.084	1.00	172.63
5	5249 5250	C	PHE D	84	47.811	55.075	32.669	1.00	140.70 140.70
J	5250 5251	ŏ	PHE D		46.952	55.941	32.546	1.00 1.00	187.78
	5252	N	SER D		48.057	54.127	31.773 30.534	1.00	187.78
	5253	CA	SER D		47.318	53.999 54.364	29.322	1.00	228.86
	5254	СВ	SER D		48.163	54.223	28.141	1.00	228.86
10	5255	OG	SER D	85	47.394 46.957	52,522	30.461	1.00	187.78
	5256	Ç	SER D	85 85	47.841	51.663	30.344	1.00	187.78
	5257	0	SER D ASP D	85 86	45.657	52.235	30.551	1.00	145.83
	5258	N	ASP D	86	45.141	50.864	30.508	1.00	145.83
15	5259	CA CB	ASP D	86	45.692	50.069	31.690	1.00	155.62
15	5260 5261	CG	ASP D	86	45.997	48.650	31.328	1.00 1.00	155.62 155.62
	5262	OD1	ASP D	86	45.107	47.971	30.755 31.610	1.00	155.62
	5263	OD2	ASP D	86	47.133	48.214	30.580	1.00	145.83
	5264	C	ASP D	86	43.621	50.885 51.914	30.878	1.00	145.83
20	5265	0	ASP D	86	43.019	49.749	30.315	1.00	152.62
	5266	N	TRP D	87	42.997 41.5 44	49.688	30.387	1.00	152.62
	5267	CA	TRP D	87 87	41.038	48.369	29.817	1.00	249.69
	5268	СВ	TRP D	87 87	40.784	48.449	28.349	1.00	249.69
05	5269	CG	TRP D	87	41.700	48.112	27.306	1.00	249.69
25	5270	CD2 CE2	TRP D	87	41.058	48.385	26.079	1.00	249.69
	5271 5272	CE3	TRP D	87	43.010	47.599	27.285	1.00	249.69 249.69
	5272 5273	CD1	TRP D	87	39.649	48.907	27.735 26.373	1.00 1.00	249.69
	5274	NE1	TRP D	87	39.807	48.868	24.845	1.00	249.69
30	5275	CZ2	TRP D	87	41.674	48.164 47.377	26.056	1.00	249.69
50	5276	CZ3	TRP D	87	43.623	47.577 47.666	24.854	1.00	249.69
	5277	CH2	TRP D	87	42.955 41.058	49.854	31.821	1.00	152.62
	5278	Ç	TRP D	87 87	40.220	50.708	32.092	1.00	152.62
۰.	5279	0	TRP D LEU D	88	41.578	49.041	32.739	1.00	136.73
35	5280	N CA	LEU D	88	41.190	49.161	34.137	1.00	136.73 120.19
	5281 5282	CB	LEU D	88	40.415	47.933	34.574	1.00 1.00	120.19
	5283	CG	LEU D	88	39.068	47.722	33.876 34.481	1.00	120.19
	5284	CD1	LEU D	88	38.314	46.521	34.012	1.00	120.19
40	5285	CD2	LEU D	88	38.232	48.972 49.364	35.043	1.00	136.73
•••	5286	C	LEU D	88	42.405	48.794	34.806	1.00	136.73
	5287	0	LEU D	88 89	43.486 42.238	50.206	36.063	1.00	129.46
	5288	N	LEU D	89	43.315	50.483	37.021	1.00	129.46
4 50	5289	CA	LEU D	89	43.867	51.888	36.838	1.00	166.27
45		CB CB	LEU D	89	44.935	52.257	37.864	1.00	166 <i>.2</i> 7 166 <i>.2</i> 7
	5291 5292	CD1	LEU D	89	46.034	51.209	37.875	1.00 1.00	166.27
	5293	CD2	LEU D	89	45.502	53.621	37.532 38.425	1.00	129.46
	5294	C	LEU D	89	42.751	50.361 50.925	38.731	1.00	129.46
50	5295	0	LEU D	89	41.706	49.611	39.278	1.00	149.29
	5296	N	LEU D	90	43.435 42.966	49.415	40.640	1.00	149.29
	5297	CA	LEU D	90 90	43.433	48.070	41.171	1.00	119.67
	5298	CB	LEU D LEU D	90	43.122	47.859	42.640	1.00	119.67
=	5299	CG CD1	LEU D	90	41.612	47.911	42.843	1.00	119.67 119.67
5:	5 5300 5301	CD2	LEU D	90	43.003	46.531	43.108	1.00	149.29
	5302	Č	LEU D	90	43.486	50.508	41.543	1.00 1.00	149.29
	5303	ŏ	LEU D	90	44.695	50.591	41.785 42.059	1.00	104.53
	5304	N	GLN D	91	42.577	51.336 52.439	42.946	1.00	104.53
6	0 5305	CA	GLN D	91	42.981	53.716	42.566	1.00	160.34
	5306	CB	GLN D	91	42.241 42.495	54.188	41.147	1.00	160.34
	5307	cG	GLN D	91 91	41.751	55.470	40.843		160.34
	5308	CD	GLN D GLN D	91	40.527	55.541	40.995		160.34
-	5309	OE1 NE2	GLN D	91	42.485	56.493	40.412		160.34 104.53
0	5 5310 5311	C	GLN D	91	42.756	52.156	44.424		104.53
	5312	ŏ	GLN D	91		51.645	44.823		107.84
	5313	Ň	ALA D			52.506	45.227 46.657		107.84
	5314	CA	ALA D	92		52.285 51.297	47.102		189.20
7	70 5315	СВ	ALA D	92	44.731	ار <u>ده</u> ا	41.10	•	

				92	43.850	53.594	47.399	1.00	107.84
	5316	C			43.683	54.436	46.987	1.00	107.84
	5317	0	ALA D SER D		43.062	53.754	48.477	1.00	115.75
	5318	N :	SER D		43.108	54.947	49.319	1.00	115.75
_	5319	CA '	SER D	93	42.212	54.756	50.553	1.00 1.00	115.29 115.29
5	5320	OG	SER D	93	42.503	53.560	51.271 49.730	1.00	115.75
	5321 5322	Č	SER D	93	44.559	55.177	49.730 49.371	1.00	115.75
	5323	ŏ	SER D	93	45.176	56.193 54.214	50.476	1.00	146.78
	5324	N	ALA D	94	45.094	54.214 54.242	50.924	1.00	146.78
10	5325	CA	ALA D	94	46.481 46.552	54.536	52.412	1.00	207.94
	5326	CB	ALA D	94 94	46.992	52.846	50.626	1.00	146.78
	5327	Ç	ALA D ALA D	94	46.194	51.905	50.566	1.00	146.78
	5328	0	GLU D	95	48.300	52.699	50.426	1.00	134.86 134.86
15	5329	N CA	GLU D	95	48.844	51.383	50.125	1.00 1.00	220.03
15	5330 5331	CB	GLU D	95	49.967	51.498	49.101 47.768	1.00	220.03
	5332	ČĞ	GLU D	95	49.489	52.026	46.687	1.00	220.03
	5333	CD	GLU D	95	50.535	51.898 52.341	45.547	1.00	220.03
	5334	OE1	GLU D	95	50.271 51.621	51.351	46.970	1.00	220.03
20	5335	OE2	GLU D	95 95	49.335	50.662	51.376	1.00	134.86
	5336	Ç	GLU D GLU D	95	49.412	49.423	51.408	1.00	134.86
	5337	0	VAL D	96	49.655	51.439	52.407	1.00	128.32 128.32
	5338	N CA	VAL D	96	50.122	50.876	53.668	1.00 1.00	128.32
25	5339	CB	VAL D	96	51.561	51.292	53.949 55.003	1.00	128.30
25	5340 5341	CG1	VAL D	96	52.157	50.377	52.675	1.00	128.30
	5342	CG2	VAL D	96	52.372	51.260 51.283	54.816	1.00	128.32
	5343	С	VAL D	96	49.242	51.383 52.588	54.932	1.00	128.32
	5344	0	VAL D	96	49.010 48.775	50.480	55.678	1.00	152.31
30	5345	N .	VAL D	97 97	47.890	50.898	56.756	1.00	152.31
	5346	CA	VAL D VAL D	97	46.438	50.575	56.406	1.00	113.44
	5347	CB CG1	VAL D	97	45.533	51.442	57.216	1.00 1.00	113.44 113.44
	5348	CG2	VAL D	97	46.185	50.774	54.941 58.152	1.00	152.31
35	5349 5350	Č	VAL D	97	48.135	50.330	58.305	1.00	152.31
55	5351	Ŏ	VAL D	97	48.616	49.193 51.133	59.160	1.00	133.53
	5352	N	MET D	98	47.765 47.880	50.784	60.590	1.00	133.53
	5353	CA	MET D	98 98	47.936	52.058	61.440	1.00	228.89
	5354	CB	MET D	98	49.145	52.951	61.220	1.00	228.89 228.89
40	5355	CG SD	MET D	98	50.627	52.296	62,005	1.00	228.89
	5356	CE	MET D	98	50.300	52.679	63.720	1.00 1.00	133.53
	5357 5358	C	MET D	98	46.651	49.985	61.010 60.868	1.00	133.53
	5359	ŏ	MET D	98	45.535	50.470	61.547	1.00	198.14
45	5360	N	GLU D	99	46.849	48.786 47.954	61.963	1.00	198.14
	5361	CA	GLU D	99	45.726 46.179	46.922	63.001	1.00	249.68
	5362	CB	GLU D	99 99	45.303	45.675	63.049	1.00	249.68
	5363	ca	GLU P	99	45.586	44.809	64.259	1.00	249.68
	5364	CD OE1	GLU D	99	46.770	44.698	64.645	1.00	249.68 249.68
50) 5365 5366	OE1	GLU D	99	44.627	44.233	64.816	1.00 1.00	198.14
	5367	C	GLU D	89	44.614	48.812	62.563 63.489		198.14
	5368	ŏ	GLU D	99		49.583 48.692	62.031	1.00	166.74
	5369	N	GLY D	100		49.467	62.569		166.74
55	5 5370	CA	GLY D	10		50.625	61.718		166.74
	5371	Ç	GLY D GLY D	10 10		51.053	61.861		166.74
	5372	0	GLN D	. 10		51.133	60.842		134.36 134.36
	5373	N CA	GLN D			52.250	59.961	1.00	207.44
6	5374 0 5375	CB	GLN D		1 43.571	52.882	59.372		207.44
O	() 5375 5376	ČĞ	GLN D			53.630	60.387 61.269		207.44
	5377	CD	GLN D			54.494 52.007	62.10		207.44
	5378	OE1	GLN D			53.987 55.807	61.08		207.44
•	5379	NE2	GLN D		01 43.607 01 41.345	51.862	58.84		134.36
6	5 5380	Ç	GLN D		01 41.345 01 41.004	50.693	58.67		134.36
	5381	0	GLN D PRO D	-	02 40.894	52.871	58.05		115.73 176.17
	5382	N CD	PRO I		02 40.996	54.307	58.28		1/6.1/
	5383 5384	CA	PRO I	-	02 39.973	52.569	58.94		176.17
•	70 5385	CB	PRO I		02 39.138	53.843	56.89	1.00	
,	, , ,								

	5386	CG	PRO D	102	40.181	54.884	57.136	1.00	176,17
	5387	č	PRO D	102	40.678	52.280	55.630	1.00	115.73
	5388	0	PRO D	102	41.771	52.810	55.342	1.00	115.73
_	5389	N	LEU D	103	40.042	51.439	54.818 52.547	1.00	118.65
5	5390	CA	LEU D	103 103	40.610 41.185	51.062 49.671	53.547 53.652	1.00 1.00	118.65 120.76
	5391 5392	CB CG	LEU D	103	42.003	49.394	52.400	1.00	120.76
	5393	CD1	LEU D	103	43.228	50.310	52.430	1.00	120.76
	5394	CD2	LEU D	103	42.399	47.938	52.323	1.00	120.76
10	5395	C	LEU D	103	39.597	51.065	52.413	1.00	118.65
	5396	0	LEU D	103	38.575	50.389 51.798	52.508 51.332	1.00 1.00	118.65 129.85
	5397 5398	N CA	PHE D PHE D	104 104	39.875 38.955	51.830	50.187	1.00	129.85
	5399	CB	PHE D	104	38.327	53.199	50.024	1.00	234.23
15	5400	ČĞ	PHE D	104	37.655	53.699	51.249	1.00	234.23
	5401	CD1	PHE D	104	38.402	54.218	52.300	1.00	234.23
	5402	CD2	PHE D	104	36.273	53.651	51.365	1.00	234.23
	5403	CE1	PHE D PHE D	104 104	37.779 35.638	54.688 54.116	53.457 52.517	1.00 1.00	234.23 234.23
20	5404 5405	CE2 CZ	PHE D	104	36.393	54.637	53.567	1.00	234.23
20	5406	Č	PHE D	104	39.651	51.480	48.881	1.00	129.85
	5407	Ö	PHE D	104	40.632	52.139	48.499	1.00	129.85
	5408	N	LEU D	105	39.152	50.446	48.198	1.00	126.08
25	5409	CA	LEU D	105	39.725	50.039	46.914	1.00	126.08
25	5410	CB CG	LEU D LEU D	105 105	40.031 41.013	48.548 48.106	46.910 47.993	1.00 1.00	130.08 130.08
	5411 5412	CD1	LEU D	105	41.358	46.640	47.803	1.00	130.08
	5413	CD2	LEU D	105	42.266	48.976	47.919	1.00	130.08
	5414	C	LEU D	105	38.719	50.360	45.832	1.00	126.08
30	5415	0	LEU D	105	37.510	50.328	46.061	1.00	126.08
	5416	N	ARG D	106	39.203	50.658	44.641	1.00	133.86
	5417	CA CB	ARG D ARG D	106 106	38.288 38.213	51.013 52.537	43.581 43.522	1.00 1.00	133.86 170.25
	5418 5419	CG	ARG D	106	37.267	53.090	42.509	1.00	170.25
35	5420	CD	ARG D	106	37.416	54.594	42.401	1.00	170.25
	5421	NE	ARG D	106	36.634	55.086	41.272	1.00	170.25
	5422	CZ	ARG D	106	36.946	56.155	40.553	1.00	170.25
	5423	NH1	ARG D	106 106	38.031 36,181	56.855 56.503	40.841 39.529	1.00 1.00	170.25 170.25
40	5424 5425	NH2 C	ARG D ARG D	106	38.732	50.439	42.239	1.00	133.86
70	5426	ŏ	ARG D	106	39.882	50.624	41.824	1.00	133.86
	5427	N	CYS D	107	37.833	49.718	41.572	1.00	163.35
	5428	ÇA	CYS D	107	38.144	49.158	40.256	1.00	163.35
45	5429	C	CYS D CYS D	107 107	37.800 36.621	50.290 50.528	39.316 39.043	1.00 1.00	1 63 .35 1 63 .35
43	5430 5431	O CB	CYS D	107	37.250	47.960	39.954	1.00	164.16
	5432	SG	CYS D	107	37.777	46,964	38.529	1.00	164.16
	5433	N	HIS D	108	38.824	50.991	38.834	1.00	196.08
	5434	CA	HIS D	108	38.626	52.153	37.962	1.00	196.08
50	5435	CB	HIS D	108	39.641	53.252	38.313 37.678	1.00	199.66
	5436 5437	CG	HIS D HIS D	108 108	39.354 40.151	54.579 55.424	37.678 36.978	1.00 1.00	199.66 199.66
	5437 5438	CD2 ND1	HIS D	108	38,135	55.214	37.796	1.00	199.66
	5439	CE1	HIS D	108	38.197	56.390	37.202	1.00	199.66
55	5440	NE2	HIS D	108	39.411	56.543	36.699	1.00	199.66
	5441	Ç	HIS D	108	38.691	51.885	36.473	1.00	196.08
	5442	0	HIS D	108	39.670	51.330 52.310	35.965 35.785	1.00 1.00	196.08 171.21
	5443 5444	N CA	GLY D	109 109	37. 63 6 37.566	52.310 52.139	34.354	1.00	171.21
60	5445	c	GLY D	109	38.291	53.283	33.690	1.00	171.21
50	5446	ŏ	GLY D	109	38.608	54.272	34.344	1.00	171.21
	5447	N	TRP D	110	38.566	53.141	32.395	1.00	191.90
	5448	CA	TRP D	110	39.258	54.181	31.637	1.00	191.90
65	5449	CB	TRP D	110	40.029	53.562 54.575	30.453 29.502	1.00	203.94 203.94
υJ	5450 5451	CG CD2	TRP D	110 110	40.592 41.946	54.575 55.053	29.502 29.444	1.00 1.00	203.94
	5452	CE2	TRP D	110	41.995	56.035	28.434	1.00	203.94
	5453	CE3	TRP D	110	43.117	54.754	30.151	1.00	203.94
=-	5454	CD1	TRP D	110	39.904	55.256	28.549	1.00	203.94
70	5455	NE1	TRP D	110	40.740	56.136	27.907	1.00	203.94

					40.470	56.718	28.110	1.00	203.94
	5456	CZ2	TRP D	110	43.173	55.439	29.823	1.00	203.94
	5457	CZ3	TRP D	110	44.291 44.305	56.406	28.809	1.00	203.94
	5458	CH2	TRP D	110 110	38.245	55.224	31.155	1.00	191.90 191.90
	5459	C	TRP D	110	37.070	54.922	30.950	1.00 1.00	162.83
5	5460	0	ARG D	111	38.715	56.454	30.987 30.568	1.00	162.83
	5461	N CA	ARG D	111	37.866	57.551	29.098	1.00	249.69
	5462	CB	ARG D	111	37.487	57.418 58.111	28.158	1.00	249.69
	5463 5464	CG	ARG D	111	38.456	58.254	26.769	1.00	249.69
10	5465	CD	ARG D	111	37.865	59.544	26.175	1.00	249.69
10	5466	NE	ARG D	111	38.203 37.865	60.717	26.705	1.00	249.69
	5467	CZ	ARG D	111 111	37.178	60.769	27.840	1.00	249.69 249.69
	5468	NH1	ARG D ARG D	111	38.209	61.844	26.098	1.00 1.00	162.83
	5469	NH2	ARG D	111	36.612	57.597	31.415 30.954	1.00	162.83
15	5470	C O	ARG D	111	35.552	58.005	32.663	1.00	190.45
	5471 5472	Ň	ASN D	112	36.744	57.175 57.162	33.595	1.00	190.45
	5473	CA	ASN D	112	35. 632 35. 30 5	53.593	34.044	1.00	228.54
	5474	CB	ASN D	112	34.442	58.632	35.296	1.00	228.54
20	5475	CG	ASN D	112 112	33.860	57.622	35.701	1.00	228.54 228.54
	5476	OD1	ASN D ASN D	112	34.352	59.805	35.914	1.00 1.00	190.45
	5477	ND2	ASN D	112	34.389	56.509	32.982 33.318	1.00	190.45
	5478	C O	ASN D	112	33.263	56.879	32.078	1.00	238.93
25	5479 5480	N	TRP D	113	34.582	55.549 54.868	31.475	1.00	238.93
25	5481	CA	TRP D	113	33.437	53.936	30.353	1.00	249.51
	5482	СВ	TRP D	113	33.872 34.087	54.608	29.061	1.00	249.51
	5483	CG	TRP D	113 113		54.251	28.071	1.00	249.51 249.51
	5484	CD2	TRP D	113		55.110	26.973	1.00 1.00	249.51
30	5485	CE2	TRP D	113		53.296	28.013 28.538	1.00	249.51
	5486	CE3 CD1	TRP D	113		55.626	27.283	1.00	249.51
	5487 5488	NE1	TRP D	113		55.940 55.038	25.816	1.00	249.51
	5489	CZ2	TRP D	113		53.222	26.864	1.00	249.51
35		CZ3	TRP D	113		54.088	25.779	1.00	249.51
,,,	5491	CH2	TRP D	113 113		54.037	32.530	1.00	238.93 238.93
	5492	C	TRP D TRP D	11		54.178	33.719	1.00 1.00	249.69
	5493	0	ASP D	11	4 31.831	53.167	32.096 33.034	1.00	249.69
40	5494	N CA	ASP D	11	4 31.117	52.312	32.843	1.00	249.69
40) 5495 5496	CB	ASP D	11		52.451 53.672	33.560	1.00	249.69
	5497	ČĞ	ASP D	11		53.780	34.798	1.00	249.69
	5498	OD1	ASP D	11		54,522	32.887	1.00	249.69
	5499	OD2	ASP D	11 11		50.845	32.895		249.69 249.69
4:	5 5500	Ç	ASP D		14 31.612	50.312	31.778		198.18
	5501	0	VAL D		15 31.825	50.203	34.032 34.043		198.18
	5502	N CA	VAL D		15 32.232	48.800	34.828		157.60
	5503 5504	CB	VAL D	1	15 33.535	48.596 47.220	34.521		157.60
5	0 5505	CG1	VAL D		15 34.102	49.673	34.470	1.00	157.60
,	5506	CG2	VAL D		15 34.539 15 31.149		34.683		198.18
	5507	Č	VAL D		15 31.149 15 30.530	40 220	35.68		198.18 134.91
	5508	0	TYR D		16 30.933	46.764	34.09		134.91
	5509	N CA	TYR		16 29.922	45.824	34 <i>.</i> 57 33.50	·	249.45
	55 5510	CB	TYR	,	16 28.849		33.50		249.45
	5511 5512	ČĞ	TYR	•	116 28.064	4	32.09		249.45
	5513	CD1	TYR	_	116 28.381	40.004	31.84	4 1.00	249.45
	5514	CE1	TYR	-	116 27.673 116 27.023		34.03	31 1.00	249.45
(60 5515	CD2		-	116 27.023 116 26.313	40 450	33.78		249.45 249.45
	5516	CE2	TYR I		116 26.83		32.60		249.45
	5517	CZ	TYR	-	116 25.93	3 50.399	32.44 34.9		134.91
	5518	C	TYR		116 30.53		34.6		134.91
	5519 65 5520	ŏ	TYR	D	116 31.70		35.6		179.36
	5521	Ň	LYS	D	117 29.73		36.0		179.36
	5522	CA	LYS		117 30.18	44.004	34.8	71 1.00	
	5523	CB	LYS	ט	117 30.27 117 28.96	40.651	34.4		
	5524	CG			117 29.20		33.6	61 1.00	249.09
	70 5525	CD	210	_					•

SSA6 CE							00.076	34.424	1.00	249.69
SSEZT NZ		EE26	CE			30.074	38.376 27.108			
SSSB				LYS D 1						179.36
5529 O LYS D 118 31.811 43.189 37.783 1.00 143.78 5530 CN VAL D 118 32.837 43.356 38.531 1.00 143.78 5531 CR VAL D 118 32.837 43.356 38.531 1.00 119.69 5532 CB VAL D 118 32.828 44.851 40.289 1.00 119.69 5533 CG2 VAL D 118 33.481 45.894 37.785 1.00 143.78 5534 CG2 VAL D 118 33.481 45.894 37.785 1.00 143.78 5535 C VAL D 118 33.481 45.894 37.785 1.00 143.78 5538 C VAL D 118 33.481 45.894 47.775 1.00 143.78 5539 C LE D 119 34.891 41.895 40.776 1.00 115.37 5539 CA ILE D 119 34.891 41.895 40.776 1.00 115.37 5539 C LE D 119 34.891 39.818 40.786 1.00 109.20 5540 CG2 ILE D 119 34.891 39.167 38.649 1.00 109.20 5541 CG1 ILE D 119 36.184 41.446 41.260 1.00 109.20 5543 C LI LE D 119 36.184 41.446 41.260 1.00 109.20 5544 C CD1 ILE D 119 37.068 41.721 40.429 1.00 109.20 5543 C LI LE D 119 37.068 41.721 40.429 1.00 109.20 5544 C CD1 ILE D 119 37.068 41.721 40.429 1.00 109.20 5544 C CB TYR D 120 37.547 41.134 41.985 42.575 1.00 109.20 5546 C CB TYR D 120 37.557 42.144 41.985 1.00 109.20 5547 C CB TYR D 120 37.557 42.144 41.985 1.00 120.348 554 C CB TYR D 120 37.557 42.144 41.985 1.00 120.32 554 554 C CB TYR D 120 37.557 42.144 41.985 1.00 120.32 555 555 C CB TYR D 120 37.557 42.144 41.985 1.00 120.32 555 555 C CB TYR D 120 37.557 42.144 41.985 1.00 120.32 555 555 C CB TYR D 120 37.557 42.144 41.985 1.00 120.32 555 555 C CB TYR D 120 37.556 41.93 41.306 1.00 120.348 555 555 C CB TYR D 120 37.556 41.93 41.306 1.00 120.348 555 555 C CB TYR D 120 37.556 41.357 41.35 555 1.00 120.32 45 555 555 C CB TYR D 120 37.556 41.357 41.357 51.00 120.32 45 555 555 C CB TYR D 120 37.556 41.357 41.357 51.00 120.348 555 556 C CB TYR D 120 37.556 41.357 41.357 51.00 120.32 45 556 556 C CB TYR D 120 37.556 41.357 41.357 51.00 120.32 45 556 556 C CB TYR D 121 30.056 555 556 C CB TYR D 121 30.056 555 557 C CB TYR D 122 41.000 122 41.000 122 41.000 122 41.000 122 41.000 122 41.000 122 41.000 122 41.000 12										
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5578					12		37.771			
5579				ASP D						
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5589							33.416			
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5592 CG GLU D 125 41.469 32.842 47.572 1.00 249.69 5594 CD GLU D 125 40.788 31.512 47.074 1.00 249.69 5594 CD GLU D 125 39.664 31.297 47.571 1.00 249.69				GLU D		25 40.682				
5584 CD GLU D 125 40.788 31.512 47.571 1.00 249.69				GLU D) 1	125 41.469				
3007				GLU C)					249.69
	ď	70 5595			י כ	125 38.00	- 01.201			

		050	GLU D	125	41.373	30.682	46.346	1.00	249.69
	5596	OE2	GLU D		39.673	35.224	44.897	1.00	141.53
	5597	C	GLU D		39.903	36.441	44.907	1.00	141.53
	5598 5599	Ň	ALA D		38.503	34.707	44.520	1.00	148.59
5	5600	ČA	ALA D		37.393	35.570	44.136	1.00	148.59
•	5601	CB	ALA D		38.274	34.743	43.560	1.00	144.26
	5602	С	ALA D		36.961	36.205	45.453 46.481	1.00 1.00	148.59 148.59
	5603	0	ALA D		36.909	35.516 37.501	45.448	1.00	169.46
	5604	N	LEU D		36.652 36.274	38.153	46,700	1.00	169.46
10	5605	CA	LEU D		37.294	39.224	47.040	1.00	146.34
	5606	CB	LEU D		37.368	39.389	48.547	1.00	146.34
	5607	CG CD1	LEU D		37.671	38.030	49.183	1.00	146.34
	5608 5609	CD2	LEU D		38.440	40.394	48.897	1.00	148.34
15	5610	C	LEU D		34.880	38.750	46.796	1.00	169.46
13	5611	ŏ	LEU D	127	34.081	38.350	47.640	1.00	169.46
	5612	N	LYS D	128	34.609	39.738	45.957	1.00 1.00	129.34 129.34
	5613	CA	LYS D	128	33.302	40.371	45.930 46.505	1.00	216.92
	5614	CB	LYS D	128	33.390	41.784 41.849	47.952	1.00	216.92
20	5615	CG	LYS D	128	33.863 32.806	41.345	48.935	1.00	216.92
	5616	CD	LYS D Lys d	128 128	33.279	41.519	50.376	1.00	216.92
	5617	CE	LYS D Lys d	128	32.194	41.270	51.366	1.00	216.92
	5618	NZ C	LYS D	128	32.834	40.419	44.475	1.00	129.34
25	5619 5620	ŏ	LYS D	128	33.645	40.314	43.556	1.00	129.34
25	5621	Ň	TYR D	129	31.532	40.581	44.261	1.00	159.52
	5622	ČA	TYR D	129	31.000	40.642	42.907	1.00	159.52
	5623	СВ	TYR D	129	30.682	39.239	42.432	1.00	146.13 146.13
	5624	CG	TYR D	129	29.763	39.234	41.246 39.958	1.00 1.00	146.13
30	5625	CD1	TYR D	129	30.255	39.420	38.859	1.00	146.13
	5626	CE1	TYR D	129	29.395 28.380	39.478 39.103	41.419	1.00	146.13
	5627	CD2	TYR D TYR D	129 129	27.507	39,162	40.337	1.00	146.13
	5628	CE2 CZ	TYR D	129	28.021	39.350	39.055	1.00	146.13
35	5629 5630	OH	TYR D	129	27.158	39.406	37. 97 6	1.00	146.13
33	5631	Č.	TYR D	129	29.747	41.516	42.767	1.00	159.52
	5632	ŏ	TYR D	129	28.858	41.489	43.622	1.00	159.52
	5633	N	TRP D	130	29.676	42.283	41.678	1.00	181.39 181.39
	5634	CA	TRP D	130	28.519	43.144	41.418 42.021	1.00 1.00	248.73
40	5635	CB	TRP D	130	28.703	44.540 44.604	43.436	1.00	248.73
	5636	CG	TRP D	130 130	29.193 28.426	44.935	44.598	1.00	248.73
	5637	CD2	TRP D	130	29.302	44.930	45.703	1.00	248.73
	5638 5639	CE2 CE3	TRP D	130	27.074	45.246	44.816	1.00	248.73
45	5640	CD1	TRP D	130	30.471	44.405	43.872	1.00	248.73
73	5641	NE1	TRP D	130	30.551	44.606	45.229	1.00	248.73
	5642	CZ2	TRP D	130	28.883	45.219	47.005	1.00	248.73 248.73
	5643	CZ3	TRP D	130	26.651	45.532	48,11 6	1.00 1.00	248.73
	5644	CH2	TRP D	130	27.555	45.511 43.326	47.192 39.916	1.00	181.39
50	5645	Ç	TRP D	130 130	28.281 29.126	43.326 42.952	39.090	1.00	181.39
	5646	0	TRP D TYR D	131	27.129	43.907	39.576	1.00	195.20
	5647	N GA	TYR D	131	26.776	44.183	38.185	1.00	195.20
	5648 5649	, CB	TYR D	131	25.263	44.162	38.020	1.00	249.67
55	5650	ČĠ	TYR D	131	24.831	44.143	36.579	1.00	249.67
33	5651	CD1	TYR D	131	24.974	42.992	35.806	1.00	249.67
	5652	CE1	TYR D	131	24.612	42.979	34.465	1.00	249.67 249.67
	5653	CD2	TYR D	131	24.311	45.285	35.973 34.632	1.00 1.00	249.67
	5654	CE2	TYR D	131	23.949	45.285	33.884	1.00	249.67
60		CZ	TYR D	131	24.101 23.751	44,131 44,140	32.553	1.00	249.67
	5656	он	TYR D	131 131	27.319	45.591	37.904	1.00	195.20
	5657	C	TYR D TYR D	131	28.458	45.746	37.468	1.00	195.20
	5658	N	GLU D	132	26.492	46.614	38.131	1.00	246.45
65	5659 5660	CA	GLU D	132	26.949	47.994	37.982	1.00	246.45
ψ.	5661	CB	GLU D	132	25.841	48.983	38.357	1.00	249.69
	5662	CG	GLU D	132	24.774	49.219	37.292	1.00	249.69
	5663	CD	GLU D	132	24.762	50.658	36.806	1.00 1.00	249.69 249.69
	5664	OE1	GLU D	132	25.408	51.508 50.945	37.461 35.777	1.00	249.69
70	5665	OE2	GLU D	132	24.106	50.945	55.777	1.00	2-70.00

		_	GLU D	132	27.976	47.929	39.090	1.00	246.45
	5666	C	GLU D	132	27.639	47.527	40.210	1.00	246.45
	5667				29.219	48.320	38.821	1.00	125.13
	5668	N	ASN D	133		48.146	39.877	1.00	125.13
_	5669	CA	ASN D	133	30.220		39.299	1.00	124.76
5	5670	CB	ASN D	133	31.670	48.261			
	5671	CG	ASN D	133	32.189	49.671	39.168	1.00	124.76
	5672	OD1	ASN D	133	31.488	50.569	38.725	1.00	124.76
	5673	ND2	ASN D	133	33.462	49.855	39.512	1.00	124.76
	5674	C	ASN D	133	30.069	48.859	41.223	1.00	125.13
10		ŏ	ASN D	133	29.046	49.479	41.527	1.00	125.13
10	5675		HIS D	134	31.077	48.688	42.057	1.00	175.64
	5676	N		134	31.054	49.259	43.375	1.00	175.64
	5677	CA	HIS D			48.218	44.358	1.00	249.69
	5678	CB	HIS D	134	30.511		45.738	1.00	249.69
	5679	CG	HIS D	134	30.264	48.759	46.925	1.00	249.69
15	5680	CD2	HIS D	134	30.834	48.440			
	5681	ND1	HIS D	134	29.361	49.759	45.988	1.00	249.69
	5682	CE1	HIS D	134	29.377	50.048	47.287	1.00	249.69
	5683	NE2	HIS D	134	30.260	49.263	47.870	1.00	249.69
	5684	Ċ	HIS D	134	32.481	49.650	43.733	1.00	175.64
20		ŏ	HIS D	134	33.352	49.738	42.862	1.00	175.64
20	5685		ASN D	135	32.714	49.878	45.020	1.00	171 <i>.2</i> 7
	5686	N	ASN D	135	34.020	50.269	45.510	1.00	171.27
	5687	CA			34.116	51.799	45.567	1.00	249.69
	5688	CB	ASN D	135		52.439	44.180	1.00	249.69
	5689	ÇG	ASN D	135	34.113			1.00	249.69
25	5690	OD1	ASN D	_. 135	34.830	51.972	43.295		
	5691	ND2	ASN D	135	33.336	53.512	43.992	1.00	249.69
	5692	С	ASN D	135	34.237	49.660	46.894	1.00	171.27
	5693	0	ASN D	135	34.009	50.303	47.907	1.00	171.27
	5694	N	ILE D	136	34.670	48.405	46.916	1.00	141.21
30	5695	CA	ILE D	136	34.953	47.636	48.143	1.00	141.21
30		CB	ILE D	136	35.894	46.432	47.813	1.00	122.14
	5696	CG2	ILE D	136	37.169	46.918	47.141	1.00	122.14
	5697			136	36.246	45.665	49.068	1.00	122.14
	5698	CG1	ILE D			44.530	48.789	1.00	122.14
	5699	CD1	ILE D	136	37.202		49.276	1.00	141.21
35	5700	С	ILE D	136	35.571	48.458		1.00	141.21
	5701	0	ile d	136	36.769	48.809	49.257		155.34
	5702	N	SER D	137	34.751	48.728	50.282	1.00	
	5703	CA	SER D	137	35.189	49.539	51.415	1.00	155.34
	5704	СВ	SER D	137	34.179	50.648	51.662	1.00	178.90
40	5705	ÖĞ	SER D	137	34.452	51.311	52.884	1.00	178.90
70		č	SER D	137	35.447	48.817	52.739	1.00	155.34
	5706	ŏ	SER D	137	34.804	47.815	53.067	1.00	155.34
	5707		ILE D	138	36.378	49.372	53.509	1.00	165.15
	5708	N		138	36.770	48.823	54.792	1.00	165.15
	5709	CA.	ILE D			48.075	54.654	1.00	128.87
45	5710	CB	ILE D	138	38.095		56.022	1.00	128.87
	5711	CG2	ILE D	138	38.690	47.804		1.00	128.87
	5712	CG1	ILE D	138	37.861	46.780	53.894		
	5713	CD1	ILE D	138	39.131	46.098	53.483	1.00	128.87
	5714	С	ILE D	138	36.919	49.901	55.863	1.00	165.15
50	5715	Ö	ILE D	138	37.703	50.849	55.720	1.00	165.15
50	5716	Ň	THR D	139	36.167	49.733	56.944	1.00	191.18
		CA.	THR D	139	36.186	50.663	58.065	1.00	191.18
	5717			139	34.891	50.533	58.855	1.00	246.32
	5718	CB	THR D		34.694	49.160	59.210	1.00	246.32
	5719	OG1	THR D	139		50.988	58.006	1.00	246.32
55	5720	CG2	THR D	139	33.713		58.976	1.00	191.18
	5721	С	THR D	139	37.364	50.342			
	5722	0	THR D	139	38.413	50.981	58.911	1.00	191.18
	5723	N	ASN D	140	37.173	49.343	59.827	1.00	193.50
	5724	CA	ASN D	140	38.211	48. 88 7	60.742	1.00	193.50
60	5725	CB	ASN D	140	37.561	48.246	61.967	1.00	183.46
-	5726	ČĠ	ASN D	140	38.567	47.701	62.943	1.00	183.46
		OD1	ASN D	140	39.474	46.972	62.554	1.00	183.46
	5727		ASN D	140	38.403	48.038	64.218	1.00	183.46
	5728	ND2			39.022	47.849	59.960	1.00	193.50
	5729	C	ASN D	140			59.482	1.00	193.50
65	5730	0	ASN D	140	38.472	46.846			163.85
	5731	N	ALA D	141	40.324	48.088	59.822	1.00	
	5732	CA	ALA D	141	41.190	47.179	59.061	1.00	163.85
	5733	CB	ALA D	141	42.181	48.002	58.187	1.00	57.61
	5734	C	ALA D	141		46.131	59.872	1.00	163.85
70	5735	Õ	ALA D	141		46.446	60.823	1.00	163.85
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			TUD D	142	41.794	44.880	59.470	1.00	158.30
	5736	N	THR D		42.464	43.765	60.113	1.00	158.30
	5737	CA	THR D	142			59.957		
	5738	CB:	THR D	142	41.654	42.471		1.00	191.01
	5739	OG1	THR D	142	40.299	42.703	60.352	1.00	191.01
5	5740	CG2	THR D	142	42.248	41.370	60.813	1.00	191.01
,	5741	Č	THR D	142	43.798	43.568	59.407	1.00	158.30
		ŏ	THR D	142	43.992	44.042	58.282	1.00	158.30
	5742			143	44.723	42.867	60.052	1.00	168.28
	5743	N .	VAL D			42.637	59.430	1.00	168.28
	5744	CA	VAL D	143	46.017				
10	5745	CB	VAL D	143	47.063	42.169	60.441	1.00	249.69
	5746	CG1	VAL D	143	46.777	40.734	60.851	1.00	249.69
	5747	CG2	VAL D	143	48.453	42.298	59.830	1.00	249.69
	5748	C	VAL D	143	45.893	41.580	58. 35 7	1.00	168.28
		ŏ	VAL D	143	46.711	41.521	57.446	1.00	168.28
	5749		OLU D	144	44.874	40.737	58.469	1.00	197.52
15	5750	N	GLU D			39.694	57.475	1.00	197.52
	5751	CA	GLU D	144	44.671		57.965	1.00	249.69
	5752	CB	GLU D	144	43.667	38.654			
	5753	CG	GLU D	144	44.088	37.957	59.232	1.00	249.69
	5754	CD	GLU D	144	43.210	38.332	60.397	1.00	249.69
20	5 755	OE1	GLU D	144	41.994	38.051	60.329	1.00	249.69
20		OE2	GLU D	144	43.729	38.910	61.376	1.00	249.69
	5756		GLU D	144	44.186	40.286	56.154	1.00	197.52
	5757	C		144	44.159	39.591	55.137	1.00	197.52
	5758	O	GLU D			41.565	56.173	1.00	135.76
	5759	N	ASP D	145	43.805			1.00	135.76
25	5760	CA	ASP D	145	43.346	42.243	54.965		
	5761	CB	ASP D	145	42.617	43.538	55.311	1.00	217.88
	5762	CG	ASP ·D	145	41.206	43.293	55.813	1.00	217.88
	5763	OD1	ASP D	145	40.415	42.658	55.081	1.00	217.88
		OD2	ASP D	145	40.881	43.737	56.938	1.00	217.88
20	5764		ASP D	145	44.512	42.549	54.030	1.00	135.76
30	5765	Ç				42.840	52.851	1.00	135.76
	5766	0	ASP D	145	44.319	42.478	54.559	1.00	129.49
	5767	N	SER D	146	45.728			1.00	129.49
	5768	CA	SER D	146	46.945	42.736	53.778		
	5769	CB	SER D	146	48.185	42.741	54.696	1.00	138.30
35	5770	OG	SER D	146	48.092	43.709	55.730	1.00	138.30
55	5771	C	SER D	146	47.128	41.662	52.709	1.00	129.49
	5772	ŏ	SER D	146	47.094	40.471	53.005	1.00	129.49
			GLY D	147	47.335	42.079	51.466	1.00	156.91
	5773	N	GLY D	147	47.534	41.109	50.400	1.00	156.91
40	5774	CA				41.750	49.041	1.00	156.91
40	5775	С	GLY D	147	47.729		48.948	1.00	156.91
	5776	0	GLY D	147	48.071	42.922			120.73
	5777	N	THR D	148	47.514	40.983	47.980	1.00	
	5778	CA	THR D	148	47.663	41.506	46.626	1.00	120.73
	5779	СВ	THR D	148	48.770	40.742	45.861	1.00	132.18
45	5780	OG1	THR D	148	48,194	39.716	45.043	1.00	132.18
43		CG2	THR D	148	49.728	40.096	46.837	1.00	132.18
	5781		THR D	148	46.320	41.438	45.848	1.00	120.73
	5782	Ç		148	45.808	40.338	45,526	1.00	120.73
	5783	0	THR D			42.618	45.545	1.00	89.32
	5784	N	TYR D	149	45.757		44.849	1.00	89.32
50	5785	CA	TYR D	149	44.471	42.706			105.54
	5786	CB	TYR D	149	43.573	43.748	45.540	1.00	
	5787	CG	TYR D	149	43.303	43.551	47.020	1.00	105.54
	5788	CD1	TYR D	149	44.281	43.842	47.984	1.00	105.54
	5789	CE1	TYR D	149	44.016	43.690	49.350	1.00	105.54
55	5790	CD2	TYR D	149	42.056	43.098	47.460	1.00	105.54
55		CE2	TYR D	149	41.781	42.942	48.812	1.00	105.54
	5791			149	42.761	43.237	49.747	1.00	105.54
	5792	CZ	TYR D			43.085	51.077	1.00	105.54
	5793	OH	TYR D	149	42.470	43.068	43.360	1.00	89.32
	5794	C	TYR D	149	44.565				89.32
60	5795	0	TYR D	149	45.586	43.579	42.877	1.00	
	5796	N	TYR D	150	43.462	42.806	42.662	1.00	127.86
	5797	CA	TYR D	150	43.278	43.117	41.246	1.00	127.86
	5798	CB	TYR D	150	44.146	42.218	40.355	1.00	148.19
		CG	TYR D	150	43.643	40.801	40.109	1.00	148.19
CF	5799		TYR D	150	42.539	40.554	39.296	1.00	148.19
65		CD1				39.243	39.025	1.00	148.19
	5801	CE1	TYR D	150			40.649	1.00	148.19
	5802	CD2	TYR D	150		39.701		1.00	148.19
	5803	CE2	TYR D	150		38.381	40.378		
	5804	ÇZ	TYR D	150		38.163	39.563	1.00	148.19
70	5805	OH	TYR D	.150	42.376	. 36.876	39.273	1.00	148.19
	2000	-							

	E000	c ·	TYR D	150	41.790	42.882	40.976	1.00	127.86
	5806 5807	ŏ	TYR D	150	41.157	42.091	41.681	1.00	127.86
	5807	N ·	CYS D	151	41.218	43.567	39.987	1.00	122.94
	5809	CA	CYS D	151	39.793	43.385	39.685	1.00	122.94
5	5610	Č	CYS D	151	39.559	43.047	38.224	1.00	122.94
5	5811	ŏ	CYS D	151	40.438	43.275	37.379	1.00	122.94
	5812	ČВ	CYS D	151	39.010	44.640	40.049	1.00	183.39
	5813	SG	CYS D	151	39.522	46.144	39.169	1.00	183.39
	5814	Ň	THR D	152	38.379	42.494	37.935	1.00	139.21
10	5815	CA	THR D	152	38.013	42.119	36. 565	1.00	139.21
	5816	СВ	THR D	152	37.955	40.598	36.383	1.00	172.57
	5817	OG1	THR D	152	36.776	40.090	37.025	1.00	172.57
	5818	CG2	THR D	152	39.185	39.945	36.985	1.00	172.57
_	5819	С	THR D	152	36.627	42.660	36.247	1.00	139.21
15	5820	0	THR D	152	35.765	42.721	37.124	1.00	139.21
	5821	N	GLY D	153	36.411	43.037	34.993	1.00	182.81
	5822	CA	GLY D	153	35.115	43.562	34.620	1.00	182.81
	5823	C	GLY D	153	34.905	43.665	33.126	1.00	182.81
•	5824	0	GLY D	153	35.844	43.520	32.350	1.00 1.00	182.81 140.36
20	5825	N	LYS D	154	33.662	43.917 44.047	32.730 31.327	1.00	140.36
	5826	CA	LYS D	154	33.307	43.211	31.040	1.00	249.69
	5827	СВ	LYS D	154 154	32.064 31.649	43.177	29.581	1.00	249.69
	5828	CG CD	LYS D LYS D	154	30.442	42.266	29.384	1.00	249.69
25	5829	CE	LYS D	154	29.973	42.264	27.938	1.00	249.69
45	5830 5831	NZ	LYS D	154	28.786	41.385	27.740	1.00	249.69
	5832	C	LYS D	154	33.055	45.519	30.936	1.00	140.36
	5833	ŏ	LYS D	154	32,150	46.184	31.458	1.00	140.36
	5834	Ň	VAL D	155	33.881	46.020	30.021	1.00	200.49
30	5835	ĊA	VAL D	155	33.793	47.390	29.517	1.00	200.49
50	5836	СВ	VAL D	155	35.198	48.038	29.434	1.00	172.58
	5837	CG1	VAL D	155	35.116	49.415	28.834	1.00	172.58
	5838	CG2	VAL D	155	35.811	48.111	30.820	1.00	172.58
	5839	С	VAL D	155	33.211	47.276	28.116	1.00	200.49
35	5840	0	VAL D	155	33.711	46.504	27.298	1.00	200.49
	5841	N	TRP D	156	32.169	48.051	27.831	1.00	193.00
	5842	CA	TRP D	156	31.502	47.986	26.522	1.00	193.00
	5843	CB	TRP D	156	32.472	48.222	25.344	1.00	249.69
40	5844	CG	TRP D	156	33.061	49.610	25.206	1.00 1.00	249.69 249.69
40	5845	CD2	TRP D	156	32.372	50.817	24.849 24.815	1.00	249.69
	5846	CE2	TRP D	156	33.330	51.857 51.121	24.550	1.00	249.69
	5847	CE3	TRP D	156	31.047	49.961	25.377	1.00	249.69
	5848	CD1	TRP D	156 156	34.372 34.537	51.309	25.141	1.00	249.69
45	5849	NE1 CZ2	TRPD	156	32.996	53.172	24.499	1.00	249.69
43	5850 5851	CZ3	TRP D	156	30.729	52.433	24.235	1.00	249.69
	5852	CH2	TRP D	156	31.692	53.438	24.219	1.00	249.69
	5853	C	TRP D	156	30.980	46.564	26.418	1.00	193.00
	5854	ŏ	TRP D	156	29.921	46.232	26.957	1.00	193.00
50	5855	Ň	GLN D	157	31.755	45. 72 7	25.732	1.00	206.01
-	5856	CA	GLN D	157	31.402	44.330	25.555	1.00	206.01
	5857	CB	GLN D	157	30.644	44.150	24.236	1.00	249.69
	5858	CG	GLN D	157	29.201	44.650	24.285	1.00	249.69
	5859	CD	GLN D	157	28.329	43.857	25,262	1.00	249.69
55	5860	OE1	GLN D	157	28.115	42.651	25.090	1.00	249.69
	5861	NE2	GLN D	157	27.820	44.535	26.291	1.00	249.69
	5862	C	GLN D	157	32.585	43.353	25.631	1.00	206.01
	5863	0	GLN D	157	32.508	42.233	25.122	1.00	206.01
	5864	N	LEU D	158	33.674	43.773	26.269	1.00	203.26 203.26
60	5865	CA	LEU D	158	34.833	42.900	26.427	1.00	242.89
	5866	CB	LEU D	158	35.991	43.350	25.529	1.00	242.89
	5867	CG	LEU D	158	35.914	43.035	24.033	1.00 1.00	242.89
	5868	CD1	LEU D	158	37.324	42.735	23.537 23.772	1.00	242.89
65	5869	CD2	LEU D	158	35.015	41.829 42.846	23.772 27.878	1.00	203.26
65	5870	C	LEU D	158	35.301 35.127	43.802	28.629	1.00	203.26
	5871	O	LEU D ASP D	158 159	35.127 35.886	43.602 41.718	28.268	1.00	176.99
	5872 5973	N CA	ASP D	159	36.376	41.545	29.629	1.00	176.99
	5873 5874	CB	ASP D	159	36.361	40.068	30.005	1.00	232.53
70	5875	CG	ASP D	159	35.012	39.424	29.781	1.00	232.53
, 0	5575	-	,				-		

	5876	OD1	ASP D	159	34.036	39.849	30.434	1.00	232.53
	5877	OD2	ASP D	159	34.929	38.495	28.950	1.00	232.53
	5878	С	ASP D	159	37.805	42.075	29.760	1.00	176.99
	5879	0	ASP D	159	38.590	42.025	28.810	1.00	176.99
5	5880	N	TYR D	160	38.143	42.588	30.938	1.00	175.60
_	5881	CA	TYR D	160	39.484	43.102	31.170	1.00	175.60
	5882	СВ	TYR D	160	39,559	44.592	30.873	1.00	205.83
	5883	CG	TYR D	160	39.112	44.956	29.483	1.00	205.83
	5884	CD1	TYR D	160	37.778	45.271	29.216	1.00	205.83
10	5885	CE1	TYR D	160	37.361	45.636	27.939	1.00	205.83
10	5886	CD2	TYR D	160	40.022	45.009	28.435	1.00	205.83
	5887	CE2	TYR D	160	39.614	45.373	27.148	1.00	205.83
	5888	CZ	TYR D	160	38.284	45.687	26.912	1.00	205.83
	5889	OH	TYR D	160	37.883	46.070	25.658	1.00	205.83
15	5890	C C	TYR D	160	39.941	42.855	32.593	1.00	175.60
13		ŏ	TYR D	160	39.151	42.853	33.545	1.00	175.60
	5891	N	GLU D	161	41.243	42.653	32.718	1.00	144.68
	5892		GLU D	161	41.879	42.385	33.998	1.00	144.68
	5893	CA	GLU D	161	42.697	41.094	33.859	1.00	232.05
20	5894	CB	GLU D		43.497	40.642	35.071	1.00	232.05
20	5895	CG		161	43.969	39.194	34. 94 2	1.00	232.05
	5896	CD	GLU D	161		38.819	35.643	1.00	232.05
	5897	OE1	GLU D	161	44.936		34.151	1.00	232.05
	5898	OE2	GLU D	161	43.363	38.430			
0.5	5899	Ç	GLU D	161	42.759	43.587	34.344	1.00	144.68
25	5900	0	GLU D	161	43.353	44.206	33.459	1.00	144.68
	5901	N	SER D	162	42.814	43.922	35.628	1.00	134.82
	5902	CA	SER D	162	43.594	45.064	36.101	1.00	134.82
	5903	CB	SER D	162	42.881	45.712	37.288	1.00	129.75
	5904	OG	SER D	162	42.767	44.801	38.381	1.00	129.75
30	5905	С	SER D	162	44.983	44.669	36.541	1.00	134.82
	5906	0	SER D	162	45.221	43.504	36.838	1.00	134.82
	5907	N	GLU D	163	45.898	45.634	36.581	1.00	145.43
	5908	CA	GLU D	163	47.238	45.334	37.050	1.00	145.43
<u>'</u> -	5909	CB	GLU D	163	48.133	46.575	36. 96 4	1.00	249.69
35	5910	CG	GLU D	163	48.587	46.949	35.552	1.00	249.69
	5911	CD	GLU D	163	49.651	46.008	35.001	1.00	249.69
	5912	OE1	GLU D	163	50.709	45.850	35.650	1.00	249.69
	5913	OE2	GLU D	163	49.433	45.429	33.917	1.00	249.69
	5914	С	GLU D	163	47.047	44.921	38.519	1.00	145.43
40	5915	0	GLU D	163	46.101	45.384	39.168	1.00	145.43
	5916	N	PRO D	164	47.906	44.037	39.057	1.00	113.31
	5917	CD	PRO D	164	48,999	43.317	38.369	1.00	144.09
	5918	CA	PRO D	164	47.794	43.578	40.447	1.00	113.31
	5919	CB	PRO D	164	48.555	42.277	40.434	1.00	144.09
45	5920	CG	PRO D'	164	49.685	42.607	39.519	1.00	144.09
	5921	C	PRO D	164	48.395	44.576	41.422	1.00	113.31
	5922	Ō	PRO D	164	49.399	45.229	41.095	1.00	113.31
	5923	Ň	LEU D	165	47.807	44.679	42.613	1.00	104.79
	5924	CA	LEU D	165	48.305	45.642	43.591	1.00	104.79
50	5925	CB	LEU D	165	47.329	46.816	43.687	1.00	127.61
50	5926	ca	LEU D	165	47,719	47.920	44.665	1.00	127.61
	5927	CD1	LEU D	165	49.250	48.130	44.649	1.00	127.61
		CD2	LEU D	165	46.959	49.193	44.283	1.00	127.61
	5928 5929	C	LEU D	165	48.560	45.097	44.980	1.00	104.79
55	5930	ŏ	LEU D	165	47.691	44.427	45.545	1.00	104.79
33	5931	Ň	ASN D	166	49.739	45.405	45.533	1.00	129.66
	5932	CA	ASN D	166	50.090	44.944	46.878	1.00	129.66
	5933	ČB	ASN D	166	51.594	44.769	47.024	1.00	189.08
			ASN D	166	52.050	43.354	46.741	1.00	189.08
60	5934	CG CD1	ASN D	166	51.275	42.407	46.867	1.00	189.08
W	5935	OD1			53.324	43.209	46.381	1.00	189.08
	5936	ND2	ASN D	166					129.66
	5937	C	ASN D	166	49.612	45.924 47.139	47.955 47.755	1.00 1.00	129.66
	5938	0	ASN D	166	49.610	47.138	47.755 40.105		129.00
"	5939	N	ILE D	167	49.221	45.387	49.105	1.00 1.00	126.98
65	5940	CA	ILE D	167	48.731	46.196	50.211		113.09
	5941	CB	ILE D	167	47.211	48.242	50.220	1.00	
	5942	CG2	ILE D	167	46.740	46.998	51.438	1.00	113.09
	5943	CG1	ILE D	167	46.716	46.889	45.940	1.00	113.09
	5944	CD1	ILE D	167	45.225	46.900	48.843	1.00	113.09
70	5945	C	ILE D	167	49.185	. 45.645	51.555	1.00	126.98

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	5040	^	ILE D	167	48.978	44.480	51.875	1.00	126.98
	5946	O N	THR D	168	49.769	46.499	52.369	1.00	123.13
	5947		THR D	168	50.238	46.029	53.647	1.00	123.13
	5948	CA	THR D	168	51.761	46.052	53.678	1.00	145.39
E	5949	CB CC1		168	52.253	45.258	52.593	1.00	145.39
5	5950	OG1	THR D		52.281	45.490	54.987	1.00	145.39
	5951	CG2	THR D	168	49.695	46.766	54.864	1.00	123.13
	5952	C	THR D	168		47.983	55.000	1.00	123.13
	5953	0	THR D	168	49.839	46.004	55.748	1.00	129.26
4.0	5954	N	VAL D	169	49.061	46.536	56.981	1.00	129.26
10	5955	CA	VAL D	169	48.501	45.982	57.209	1.00	119.28
	5956	CB	VAL. D	169	47.067		58.653	1.00	119.28
	5 95 7	CG1	VAL D	169	46.683	46.096		1.00	119.28
	5958	CG2	VAL D	169	46.065	46.769	56.377		
	5959	С	VAL D	169	49.439	46.104	58.098	1.00	129.26
15	5960	0	VAL D	169	49.525	44.914	58.419	1.00	129.26 108.63
	5961	N	ILE D	170	50.162	47.069	58.664	1.00	
	5962	CA	ILE D	170	51.111	46.798	59.750	1.00	108.63
	5963	CB	ILE D	170	52.340	47.687	59.607	1.00	169.72
	5964	CG2	ILE D	170	52.891	47.560	58.200	1.00	169.72
20	5965	CG1	ILE D	170	51.963	49.148	59.833	1.00	169.72
	5966	CD1	ILE D	170	53.138	50.116	59.741	1.00	169.72
	5967	С	ILE D	170	50.448	47.058	61.111	1.00	108.63
	5968	0	ILE D	170	49.389	47.687	61.170	1.00	108.63
	5969	N	LYS D	171	51.044	46.600	62.206	1.00	180.64
25	5970	CA	LYS D	171	50.427	46.811	63.518	1.00	180.64
25	5971	CB	LYS D	171	50.095	45.460	64.130	1.00	216.97
	5972	CG	LYS D	171	51.300	44.550	64.204	1.00	216.97
	5973	CD	LYS D	171	50.911	43.084	64.180	1.00	216.97
	5974	CE	LYS D	171	49.997	42.721	65.338	1.00	216.97
30	5975	NZ	LYS D	171	49.677	41.265	65.351	1.00	216.97
50	5976	Ċ	LYS D	171	51.277	47.623	64.496	1.00	180.64
	5977	ŏ	LYS D	171	50.952	47.715	65.686	1.00	180.64
	5978	C1	NAG D	221	40.588	68.345	34.460	1.00	249.69
	5979	čž	NAG D	221	39.263	67.620	34,228	1.00	249.69
35	5980	N2	NAG D	221	39.503	68.190	34.156	1.00	249.69
23	5981	C7	NAG D	221	38.524	65.328	34.426	1.00	249.69
	5982	07	NAG D	221	37.379	65.680	34.734	1.00	249.69
	5983	C8	NAG D	221	38.865	63.847	34.336	1.00	249.69
	5984	ä	NAG D	221	38.607	68.107	32.935	1.00	249.69
40	5985	õ	NAG D	221	37.303	67.542	32.815	1.00	249.69
40	5986	24	NAG D	221	38.508	69.645	32.882	1.00	249.69
		54	NAG D	221	38.122	70.004	31.534	1.00	249.69
	5987 5988	C5	NAG D	221	39.874	70.288	33.238	1.00	249.69
	5989	O5	NAG D	221	40.374	69.764	34.489	1.00	2 (9.69
45		C6	NAG D	221	39.806	71.797	33.398	1.00	249.69
43	5990	O6	NAG D	221	38.830	72.175	34,359	1.00	249.69
	5991	C1	NAG D	222	37.598	71.265	31.271	1.00	249.69
	5992		NAG D	222	36.393	71.128	30.316	1.00	249.69
	5993	C2	NAG D	222	35.353	70.322	30.940	1.00	249.69
50	5994	N2		222	34.138	70.826	31.159	1.00	249.69
50	5995	C7		222	33.821	71.980	30.854	1.00	249.69
	5996	07	NAG D		33.115	69.911	31.816	1.00	249.69
	5997	C8	NAG D	222	36.853	70.476	28.991	. 1.00	249.69
	5998	cs	NAG D	222		70.461	28.055	1.00	249.69
	5999	03	NAG D	222	35.784	71.236	28.392	1.00	249.69
55	6000	C4	NAG D	222	38.047	71.236 70.527	27.265	1.00	249.69
	6001	04	NAG D	222	38.552		29,445	1.00	249.69
	6002	C5	NAG D	222	39.161	71.402	30.639	1.00	249.69
	6003	O 5	NAG D	222	38.632	72.044	28.961	1.00	249.69
	6004	C 6	NAG D	222	40.342	72.235	29.216	1.00	249.69
60		06	NAG D	222	41.578	71.582	29.210		217.32
	6006	C1	NAG D	242	60.393	61.563	38.161	1.00	217.32
	6007	C2	NAG D	242	60.080	62.065	36.753	1.00	
	6008	N2	NAG D	242	59.542	63.410	36.776	1.00	217.32
	6009	C7	NAG D	242	60.185	64.390	36.140	1.00	217.32
65		07	NAG D	242	61.243	64.215	35.527	1.00	217.32
	6011	C8	NAG D	242	59.572	65.781	36.193	1.00	217.32
	6012	СЗ	NAG D	242	59.090	61.109	36.102	1.00	217.32
	6013	03	NAG D	242	58.789	61.543	34.778	1.00	217.32
	6014	C4	NAG D	242		59. 697	36.072	1.00	217.32
70	6015	04	NAG D	242	58.682	58.764	35.604	1.00	217.32

						F0 070	07.475	1.00	047.00
	6016	C5	NAG D	242	60.173	59.270	37.475	1.00	217.32
	6017	Q 5	NAG D	242	61.023	60.283	38.071	1.00	217.32
	6018	C6	NAG D	242	61,001	57.999	37.419	1.00	217.32
_	6019	Q6	NAG D	242	60.329	56.906 58.907	38.029 34.449	1.00 1.00	217.32
5	6020	C1	NAG D	243	58.975	58.047 56.797	34.373	1.00	249.32 249.32
	6021	C2	NAG D	243	58.093	55.934	35.517	1.00	249.32 249.32
	6022	N2	NAG D	243	58.304	55.458	36.184	1.00	249.32
	6023	C7	NAG D	243	57.260	55.727	35.887	1.00	249.32
	6024	07	NAG D	243	56.095 57.553	54.550	37.368	1.00	249.32
10	6025	C8	NAG D	243 243	58.410	56.048	33.091	1.00	249.32
	6026	C3	NAG D NAG D	243	57.609	54.878	32.999	1.00	249.32
	6027	O3 C4	NAG D	243	58.125	56.960	31,920	1.00	249.32
	6028	04	NAG D	243	58.387	56.198	30.758	1.00	249.32
15	6029	C5	NAG D	243	58.994	58.245	32.040	1.00	249.32
13	6030	O5	NAG D	243	58.710	58.893	33.315	1.00	249.32
	6031 6032	C6	NAG D	243	58.695	59.274	30.969	1.00	249.32
	6033	06	NAG D	243	57.361	59.747	31.063	1.00	249.32
	6034	C1	MAN D	244	57.701	56.400	29.591	1.00	249.69
20	6035	C2	MAN D	244	58.764	56.236	28.599	1.00	249.69
20	6036	02	MAN D	244	59.572	55.101	28.964	1.00	249.69
	6037	C3	MAN D	244	58.183	56.214	27.213	1.00	249.69
	6038	.03	MAN D	244	59.205	56.198	26.236	1.00	249.69
	6039	C4	MAN D	244	57.187	55.086	27.057	1.00	249.69
25	6040	O4	MAN D	244	56.690	55.063	25.730	1.00	249.69
	6041	C5	MAN D	244	56.059	55.334	28.066	1.00	249.69
	6042	O5	MAN D	244	56.637	55.331	29.433	1.00	249.69
	6043	C6	MAN D	244	54.855	54.371	27.914	1.00	249.69
	6044	O6	MAN D	244	55.056	53.129	28.567 45.348	1.00 1.00	249.69 249.69
30	6045	C1	NAG D	250	45.970	78.192 78.482	45.867	1.00	249.69
	6046	C2	NAG D	250 250	44.549 44.538	78.485	47.317	1.00	249.69
	6047	N2	NAG D NAG D	250 250	44.384	79.627	47.981	1.00	249.69
	6048	C7 O7	NAG D	250	44.241	80.713	47.415	1.00	249.69
35	6049 6050	C8	NAG D	250	44.386	79.553	49.506	1.00	249.69
33	6051	C3	NAG D	250	43.581	77.413	45.337	1.00	249.69
	6052	03	NAG D	250	42.249	77.716	45.732	1.00	249.69
	6053	C4	NAG D	250	43.666	77.341	43.807	1.00	249.69
	6054	04	NAG D	250	42,863	76.265	43.339	1.00	249.69
40	6055	C5	NAG D	250	45.136	77.138	43.368	1.00	249.69
	6056	O5	NAG D	250	45.975	78.187	43.916	1.00	249.69
	6057	C6	NAG D	250	45.334	77.155	41.856	1.00 1.00	249.69 249.69
	6058	O 6	NAG D	250	46.706	77.343	41.513 61.817	1.00	249.69
40	6059	C1	NAG D	274	64.018	69.436 68.308	62.845	1.00	249.69
45	6060	C2	NAG D	274 274	63.805 62.614	68.567	63,639	1.00	249.69
	6061	N2 C7	NAG D NAG D	274	61.945	67.559	64.201	1.00	249.69
	6062 6063	07 07	NAG D	274	62.289	68.377	64,093	1.00	249.69
	6064	C8	NAG D	274	60.707	67.911	65.011	1.00	249.69
50	6065	cs	NAG D	274	65.040	68.194	63.760	1.00	249.69
30	6066	Ö	NAG D	274	64.908	67.066	64.619	1.00	249.69
	6067	C4	NAG D	274	66.321	68.053	62.922	1.00	249.69
	6068	Ö 4	NAG D	274	67.463	68.083	63.776	1.00	249.69
	6069	C5	NAG D	274	66.405	69.191	61.890	1.00	249.69
55	6070	O5	NAG D	274	65.217	69.199	61.060	1.00	249.69
	6071	C6	NAG D	274	67.605	69.054	60.964	1.00	249.69
	6072	O6	NAG D	274	67.558	70.006	59.911	1.00	249.69
	6073	C1	NAG D	335	33.933	54.753	43.517	1.00	249.69 249.69
60	6074	C2	NAG D	335	33.681	55.966 EE 476	44.462 45.707	1.00 1.00	249.69
60	6075	N2	NAG D	335	33.369 34.175	55.476 55.736	45,797 46,826	1.00	249.69
	6076	C7	NAG D	335 335	35.208	56.398	46.727	1.00	249.69
	6077	O7	NAG D	335	33.768	55.178	48.177	1.00	249.69
	6078 6079	C8 C3	NAG D NAG D	335	32.547	56.909	44.003	1.00	249.69
65	6080	03	NAG D	335	32.693	58.170	44.644	1.00	249.69
5 5	6081	Ç4	NAG D	335	32.568	57.114	42.494	1.00	249.69
	6082	04	NAG D	335	31.469	57.925	42.098	1.00	249.69
	6083	C5	NAG D	335	32.490	55.747	41.830	1.00	249.69
	6084	O 5	NAG D	335	33.699	55.014	42.109	1.00	249.69
70	6085	C6	NAG D	335	32.365	55.844	40.319	1.00	249.69

	6086	00	N40 D						
	6087	O6 C1	NAG D NAG D	335 340	31.232	55.131	39.850	1.00	249.69
	6088	C2	NAG D	340	38.129 39.319	47.005	65.199	1.00	249.69
	6089	N2	NAG D	340	40.524	46.805 46.521	66.150	1.00	249.69
5	6090	C7	NAG D	340	41.665	47.160	65.388 65.655	1.00	249.69
	6091	07	NAG D	340	41.779	48.007	66.549	1.00 1.00	249.69
	6092	C8	NAG D	340	42.871	46.799	64.801	1.00	249.69
	6093	C3	NAG D	340	39.000	45.640	67.106	1.00	249.69 249.69
10	6094	O3	NAG D	340	40.042	45.482	68.064	1.00	249.69
10	6095	C4	NAG D	340	37.670	45.894	67.828	1.00	249.69
	6096	04	NAG D	340	37.324	44.743	68.593	1.00	249.69
	6097 6098	C5 O5	NAG D	340	36.556	46.207	66.801	1.00	249.69
	6099	C6	NAG D NAG D	340 340	36.949	47.307	65.948	1.00	249.69
15	6100	06	NAG D	340	35.226 34.319	46.591 47.067	67.427	1.00	249.69
	6101	C1	NAG D	366	53.829	41.917	66.440 45. 964	1.00 1.00	249.69
	6102	C2	NAG D	366	54.811	42.093	44.812	1.00	214.56
	6103	N2	NAG D	366	54.141	42.757	43.705	1.00	214.56 214.56
00	6104	C7	NAG D	366	54.172	44.086	43.595	1.00	214.56
20	6105	07	NAG D	366	54.769	44.819	44.396	1.00	214.56
	6106	C8	NAG D	366	53.436	44.705	42.413	1.00	214.56
	6107 6108	C3 O3	NAG D	366	55.328	40.725	44.367	1.00	214.56
	6109	03 C4	NAG D NAG D	366 366	56.374	40.896	43.416	1.00	214.56
25	6110	04	NAG D	366	55.847 56.067	39.896 38.537	45.553	1.00	214.56
	6111	C5	NAG D	366	54.830	39.900	45.104 46.709	1.00 1.00	214.56
	6112	O5	NAG D	366	54.471	41.245	47.050	1.00	214.56
	6113	C6	NAG D	366	55.334	39.248	47.980	1.00	214.56 214.56
20	6114	O6	NAG D	366	54.292	39.118	48.934	1.00	214.56
30	6115	C1	NAG D	367	57.323	37.987	45.329	1.00	231.83
	6116 6117	C2 N2	NAG D	367	57.238	36.462	45.283	1.00	231.83
	6118	C7	NAG D NAG D	367 367	56.271	35.974	46.246	1.00	231.83
	6119	O7	NAG D	367	55.141 54.861	35.410 35.279	45.821 44.620	1.00	231.83
35	6120	C8	NAG D	367	54.169	34.918	46.887	1.00 1.00	231.83 231.83
	6121	C3	NAG D	367	58.627	35.898	45.572	1.00	231.83
	6122	O3	NAG D	367	58.601	34.478	45.528	1.00	231.83
	6123	C4	NAG D	367	59.611	36.433	44.526	1.00	231.83
40	6124 6125	O4 C5	nag d Nag d	367	60.922	35.989	44.845	1.00	231.83
40	6126	O5	NAG D	367 367	59.572 58.216	37.974	44.486	1.00	231.83
	6127	C6	NAG D	367	60.403	38.443 38.550	44.296 43.358	1.00	231.83
	6128	O6	NAG D	367	59.584	39.177	42.385	1.00 1.00	231.83
	6129	CB	LYS E	4	8.883	64.586	0.000	1.00	231.83 249.69
45	6130	CG	LYS E	4	7.510	64.141	-0.503	1.00	249.69
	6131	CD	LYS E	4	6.532	63.873	0.645	1.00	249.69
	6132 6133	CE	LYS E	4	5.149	63.459	0.123	1.00	249.69
	6134	NZ C	LYS E LYS E	4	4.173	63.179	1.220	1.00	249.69
50	6135	ŏ	LYS E	4	9.271 8.420	66.045 66.812	-1.989	1.00	232.34
	6136	Ň	LYS E	4	11.173	65.351	-1.537 -0.540	1.00 1.00	232.34 232.34
	6137	CA	LYS E	4	9.885	64.939	-1.121	1.00	232.34
	6138	N	PRO E	5	9.723	66.150	-3.249	1.00	227.45
55	6139	CD	PRO E	5	10.890	65.481	-3.843	1.00	124.73
33	6140	CA	PRO E	5	9.204	67.180	-4.150	1.00	227.45
	6141 6142	CB CG	PRO E	5	10.351	67.382	-5.132	1.00	124.73
	6143	C	PRO E PRO E	5 .	10.883	66.000	-5 .27 5	1.00	124.73
	6144	ŏ	PRO E	5 5	7.921 7.651	66.721 65.522	-4.845 4.054	1.00	227.45
60	6145	N	LYS E	6	7.125	67.679	-4.954 -5.305	1.00 1.00	227.45 237.93
	6146	CA	LYS E	6	5.877	67.360	-5.987	1.00	237.93 237.93
	6147	CB	LYS E	6	4.702	67.440	-5.011	1.00	249.69
	6148	CG	LYS E	6	3.370	67.066	-5.640	1.00	249.69
65	6149	CD	LYS E	6	2.244	66.993	-4.615	1.00	249.69
UJ	6150	CE	LYS E	6	0.935	66.562	-5 <i>.2</i> 75	1.00	249.69
	6151 6152	NZ C	LYS E LYS E	6	-0.156 5.650	68.352	-4.287	1.00	249.69
	6152 6153	ŏ	LYS E	6 6	5.650 5.422	68.308 69.505	-7.153 c.070	1.00	237.93
	6154	Ň	VAL E	7	5.709	69.505 67.754	-6.970 -8.356	1.00	237.93
70	6155	CA	VAL E	7	5.532	68.543	-0.330 -9.567	1.00 1.00	162.26 162.26
									102.20

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	6156	СВ	VAL E	7 .	5.858	67.703	10 001	4.00	
	6157	CG1	VAL E	7	6.017	68.614	-10.821 -12.040	1.00 1.00	205.67
	6158	CG2	VAL E	7	7.117	66.881	-10,577	1.00	205.67 205.67
_	6159	C	VAL E	7	4.118	69.111	-9.723	1.00	162.26
5	6160	0	VAL E	7	3.134	68.364	-9.717	1.00	162.26
	6161	N	SER E	8	4.022	70.433	-9.868	1.00	174.49
	6162	CA	SER E	8	2.741	71.111	-10.048	1.00	174.49
	6163	CB	SER E	8	2.672	72.324	-9.131	1.00	223.27
10	6164 6165	OG C	SER E	8	3.850	73.111	-9.231	1.00	223.27
10	6166	ŏ	SER E SER E	8 8	2.616 3.624	71.551	-11.501	1.00	174.49
	6167	Ň	LEU E	9	1.392	71.640 71.815	-12.215 -11.949	1.00	174.49
	6168	ĊA	LEU E	9	1.200	72.248	-13.338	1.00 1.00	138.24
	6169	CB	LEU E	9	0.497	71.161	-14.181	1.00	138.24 151.07
15	6170	CG	LEU E	9	1.092	69.761	-14.372	1.00	151.07
	6171	CD1	LEU E	9	0.374	69.105	-15.529	1.00	151.07
	6172	CD2	LEU E	9	2.578	69.816	-14.665	1.00	151.07
	6173	C	LEU E	9	0.394	73.544	-13.447	1.00	138.24
20	6174 6175	0	LEU E	9	-0.329	73.919	-12.519	1.00	138.24
20	6176	N CA	ASN E ASN E	10 10	0.520	74.217	-14.589	1.00	163.51
	6177	CB	ASN E	10	-0.215 0.444	75.436 76.592	-14.823 -14.100	1.00	163.51
	6178	CG	ASN E	10	-0.467	77.788	-14.008	1.00 1.00	242.89
	6179	OD1	ASN E	10	-1.520	77.730	-13.369	1.00	242.89 242.89
25	6180	ND2	ASN E	10	-0.077	78.881	-14.650	1.00	242.89
	6181	С	ASN E	10	-0.303	75.748	-16.310	1.00	163.51
	6182	0	ASN E	10	0.703	76.073	-16.942	1.00	163.51
	6183	N	PRO E	11	-1.515	75.661	-16.902	1.00	167.75
30	6184 6185	CD CA	PRO E PRO E	11	-1.686	75.947	-18.332	1.00	141.15
50	6186	CB	PRO E	11 11	-2.807 -3.740	75.308	-16.289	1.00	167.75
	6187	CG	PRO E	11	-3.740 -3.151	75.243 76.257	-17.494 -18.413	1.00 1.00	141.15
	6188	Ċ_	PRO E	ii	-2.804	73.994	-15.505	1.00	141.15 167.75
	6189	0	PRO E	11	-1.861	73,210	-15.588	1.00	167.75
35	6190	N	PRO E	12	-3.874	73.7 3 6	-14.729	1.00	129.01
	6191	CD	PRO E	12	-5.008	74.630	-14.438	1.00	158.46
	6192 6193	CA	PRO E	12	-3.963	72.506	-13.934	1.00	129.01
	6194	CB CG	PRO E PRO E	12 12	-5.164	72.766	-13.028	1.00	158.46
40	6195	č	PRO E	12	-5. 297 -4.198	74.281 71.307	-13.015	1.00	158.46
	6196	ŏ	PRO E	12	-3.823	70.178	-14.852 -14.535	1.00 1.00	129.01
	6197	N	TRP E	13	-4.829	71.590	-15.992	1.00	129.01 148.97
	6198	CA	TRP E	13	-5.176	70.617	-17.041	1.00	148.97
45	6199	СВ	TRP E	13	-5.707	71.376	-18.252	1.00	139.57
45	6200	CG	TRP E	13	-6.745	72.405	-17.878	1.00	139.57
•	6201 6202	CD2 CE2	TRP E	13	-7.685	72.310	-16.810	1.00	139.57
	6203	CE3	TRP E	13 13	-8.485 -7.934	73.479	-16.851	1.00	139.57
	6204	CD1	TRP E	13	-7.006	71.351 73.598	-15.816	1.00	139.57
50	6205	NE1	TRP E	13	-8.049	74.249	-18.513 -17.900	1.00 1.00	139.57 139.57
	6206	CZ2	TRP E	13	-9.511	73.707	-15,934	1.00	139.57
	6207	CZ3	TRP E	13	-8.950	71.581	-14.909	1.00	139.57
	6208	CH2	TRP E	13	-9.731	72.746	-14.975	1.00	139.57
55	6209	C	TRP E	13	-4.000	69.772	-17.478	1.00	148.97
33	6210 6211	O _N	TRP E	13	-3.050	70.294	-18.052	1.00	148.97
	6212	N CA	ASN E	14 14	-4.069 -2.067	68.465	-17.236	1.00	121.67
	6213	CB	ASN E	14	-2.967 -2.569	67.569 66.659	-17. 623 -16.443	1.00	121.67
	6214	CG	ASN E	14	-3.669	65.717	-16.039	1.00 1.00	170.43 170.43
60	6215	OD1	ASN E	14	-4.785	68.134	-15.711	1.00	170.43
	6216	ND2	ASN E	14	-3.382	64.432	-16.058	1.00	170.43
	6217	C	ASN E	14	-3.273	66.730	-18.871	1.00	121.67
	6218	0	ASN E	14	-2.662	65.684	-19.103	1.00	121.67
65	6219 6220	N CA	ARG E	15	-4.227	67.225	-19.661	1.00	100.94
05	6221	CA CB	ARG E ARG E	15 15	-4.675 -6.060	66.616 65.001	-20.914	1.00	100.94
	6222	ČĠ	ARG E	15	-6.069 -6.278	65.991 65.052	-20.773 -19.581	1.00	110.25
	6223	CD	ARG E	15	-7. 642	64.353	-19.561 -19.673	1.00 1.00	110.25 110.25
=-	6224	NE	ARG E	15	-7.673	63.268	-20.667	1.00	110.25
70	6225	CZ	ARG E	15	-8.713	62.965	-21.449	1.00	110.25

	6226	NH1	ARG E	15	-9.818	63.665	-21.363	1.00	110,25
	6227	NH2	ARG E	15	-8.654	61.949	-22.308	1.00	110.25
	6228	C	ARG E	15	-4.797	67.800	-21.845	1.00	100.94
5	6229 6230	O N	ARG E ILE E	15	-5.779	68.526	-21.776	1.00	100.94
9	6231	CA	ILE E	16 16	-3.824 -3.875	68.012	-22.720	1.00	114.46
	6232	CB	ILE E	16	-3.873 -2.723	69.182 70.141	-23.615 -23.315	1.00	114.48
	6233	CG2	ILE E	16	-3.008	70.920	-22.025	1.00 1.00	133.29
	6234	CG1	ILE E	16	-1.422	69.334	-23.257	1.00	133.29 133.29
10	6235	CD1	ILE E	16	-0.187	70.169	-23.241	1.00	133.29
	6236	С	ILE E	16	-3.835	68.931	-25.116	1.00	114.46
	6237	0	ILE E	16	-3.314	67.920	-25.573	1.00	114.46
	6238	N	PHE E	17	-4.371	69.884	-25.869	1.00	157.55
15	6239 6240	CA CB	PHE E PHE E	17	-4.389	69.799	-27.315	1.00	157.55
13	6241	CG	PHE E PHE E	17 17	-5.291 -6.708	70.875	-27.896	1.00	134.86
	6242	CD1	PHE E	17	-0.708 -7.747	70.444 71.354	-28.068 -27.884	1.00 1.00	134.86
	6243	CD2	PHE E	17	-7.016		-28.445	1.00	134.86 134.86
	6244	CE1	PHE E	17	-9.085	70.974	-28.072	1.00	134.86
20	6245	CE2	PHE E	17	-8.339	68.753	-28.636	1.00	134.86
	6246	CZ	PHE E	17	-9.378	69.677	-28.448	1.00	134.86
	6247	C	PHE E	17	-2.984	69.975	-27.873	1.00	157.55
	6248 6249	O N	PHE E	17	-2.038	70.221	-27.122	1.00	157.55
25	6250	CA	LYS E	18 18	-2.860	69.858	-29.196	1.00	136.71
	6251	CB	LYS E	18	-1.582 -1.660	69.998 69.250	-29.892 -31.219	1.00	136.71
	6252	ČĞ	LYS E	18	-0.384	69.249	-31.219	1.00 1.00	249.69
	6253	CD	LYS E	18	-0.530	68.316	-33.230	1.00	249.69 249.69
	6254	CE	LYS E	18	0.701	68.337	-34.128	1.00	249.69
30	6255	NZ	LYS E	18	0.855	69.643	-34.825	1.00	249.69
	6256	C	LYS E	18	-1.243	71.471	30.127	1.00	136.71
	6257 6258	0 N	LYS E GLY E	18	-2.056	72.237	-30.646	1.00	136.71
	6259	CA	GLY E	19 19	-0.042 0.380	71.866	-29.726	1.00	201.41
35	6260	č	GLY E	19	0.380	73.242 74.161	-29.913 -28.717	1.00 1.00	201.41
	6261	Ŏ	GLY E	19	0.717	75.279	-28.708	1.00	201.41 201.41
	6262	N	GLU E	20	-0.541	73.703	-27.709	1.00	148.40
	6263	CA	GLU E	20	-0.787	74.499	-26.497	1.00	148.40
40	6264	CB	GLU E	20	-2.004	73.945	-25. 733	1.00	165.83
40	6265 6266	CG	GLU E	20	-3.267	73.658	-26.577	1.00	165.83
	6267	OE1	GLU E	20 20	-4.479 -4.358	73.233 72.282	-25.726	1.00	165.83
	6268	OE2	GLU E	20	-5.555	73.855	-24.926 -25.864	1.00 1.00	165.83 165.83
	6269	C	GLU E	20	0.439	74.469	-25.564	1.00	148.40
45	6270	0	GLU E	20	1.273	73.561	-25.663	1.00	148.40
	6271	N	ASN E	21	0.552	75.440	-24.653	1.00	156.11
	6272	CA	ASN E	21	1.704	75.474	-23.731	1.00	156.11
	6273 6274	CB CG	ASN E	21	2.412	76.835	-23.774	1.00	249.69
50	6275	OD1	ASN E ASN E	21 21	2.414	77.468	-25.153	1.00	249.69
-	6276	ND2	ASN E	21	2.734 2.070	76.825 78.754	-26.157 -25.179	1.00 1.00	249.69
	6277	C	ASN E	21	1.342	75.182	-22.267	1.00	249.69
	6278	تَ	ASN E	21	0.288	75.589	-21.769	1.00	156.11 / 156.11 [/]
	6279	N	VAL E	22	2.245	74.493	-21.580	1.00	182.17
55	6280	CA	VAL E	22	2.049	74.137	-20.177	1.00	182.17
	6281	CB	VAL E	22	1.601	72.669	-20.028	1.00	148.81
	6282 6283	CG1	VAL E	22	2.757	71.742	-20.356	1.00	148.81
	6284	CG2 C	VAL E VAL E	22 22	1.109 3.360	72.404	-18.627	1.00	148.81
60	6285	ŏ	VAL E	22	4.443	74.313 74.124	-19.407	1.00	182.17
	6286	Ň	THR E	23	3.261	74.650	-19.965 -18.120	1.00 1.00	182.17 131.37
	6287	CA	THR E	23	4.447	74.874	-17.281	1.00	131.37
	6288	СВ	THR E	23	4.448	76.320	-16.723	1.00	249.69
65	6289	OG1	THR E	23	4.251	77.255	-17.794	1.00	249.69
65	6290	CG2	THR E	23	5.773	76.619	-16.027	1.00	249.69
	6291	C	THR E	23	4.559	73.928	-16.088	1.00	131.37
	6292 6293	0 N	THR E LEU E	23 24	3.643	73.866	-15.266	1.00	131.37
	6294	CA	LEU E	24	5.694 5.909	73.234 72.305	-15.974 -14.862	1.00	247.08
70	6295	CB	LEU E	24	6.490	72.305 70.972	-14.862 -15.357	1.00 1.00	247.08 141.93
				•	100			1.00	141.50

	cooe	00		٠.	0.454	70.407			
	6296 6297	CG CD1	LEV E	24 ⁻ 24	6.154 6.601	70.407 68.946	-16.745	1.00	141.93
	6298	CD2	LEU E	24	4.668	70.513	-16.814 -17.025	1.00	141.83
	6299	C	LEU E	24	6.857	72.886	-13.807	1.00 1.00	141.93
5	6300	Ö	LEU E	24	8.064	72.988	-14.032	1.00	247.08 247.08
	6301	N	THR E	25	6.302	73.254	-12.653	1.00	187.47
	6302	CA	THR E	25	7.075	73.824	-11.547	1.00	187.47
	6303	CB	THR E	25	6.280	74.957	-10.847	1.00	161.19
10	6304	OG1	THR E	25	5.936	75.964	-11.806	1.00	161.19
10	6305	CG2	THR E	25	7.100	75.590	-9.725	1.00	161.19
	6306 6307	c o	THR E	25 25	7.391 6.513	72.739	-10.512	1.00	187.47
	6308	Ň	CYS E	25 26	8.642	71.981 72.673	-10.121 -10.069	1.00 1.00	187.47
	6309	CA	CYS E	26	9.057	71.677	-9.078	1.00	208.94 208.94
15	6310	C	CYS E	26	8.680	72.137	-7. 667	1.00	208.94
	6311	0	CYS E	26	8.738	73.326	-7.364	1.00	208.94
	6312	CB	CYS E	26	10.562	71.439	-9.179	1.00	205.14
	6313	SG	CYS E	26	11.190	70.046	-8.197	1.00	205.14
20	6314 6315	N CA	ASN E	27	8.303	71.189	-6.812	1.00	249.69
20	6316	CB	ASN E ASN E	27 27	7.875 8.415	71.478	-5.439	1.00	249.69
	6317	CG	ASN E	27 27	7.792	70.418 70.526	-4.468 -3.076	1.00 1.00	249.69
	6318	OD1	ASN E	27	6.569	70.623	-2.936	1.00	249.69 249.69
	6319	ND2	ASN E	27	8.632	70.505	-2.043	1.00	249.69
25	6320	С	ASN E	27	8.241	72.870	-4.930	1.00	249.69
	6321	0	ASN E	27	9.333	73.095	-4.401	1.00	249.69
	6322	N	GLY E	28	7.301	73.795	-5.095	1.00	249.69
	6323	CA	GLY E	28	7.486	75.172	-4.669	1.00	249.69
30	6324 6325	CO	GLY E	28	6.306	75.960	-5.202	1.00	249.69
30	6326	Ň	ASN E	28 29	6.092 5.537	76.005 76.576	-6.419 4.205	1.00	249.69
	6327	CA	ASN E	29	4.349	75.376 77.334	-4.305 -4.702	1.00 1.00	249.69
	6328	CB	ASN E	29	3.447	77.573	-3.470	1.00	249.69 249.69
	6329	CG	ASN E	29	2.043	78.092	-3.837	1.00	249.69
35	6330	OD1	ASN E	29	1.664	78.143	-5.013	1.00	249.69
	6331	ND2	ASN E	29	1.268	78.469	-2.821	1.00	249.69
	6332	C	ASN E	29	4.659	78.665	-5.406	1.00	249.69
	6333 6334	O N	ASN E	29	4.147	78.925	-6.509	1.00	249.69
40	6335	CA	ASN E	30 30	5.502 5.807	79.498 80.792	-4.796 -5.395	1.00 1.00	249.69
	6336	CB	ASN E	30	5.157	81.904	-3.395 -4.559	1.00	249.69 249.69
	6337	CG	ASN E	30	3.636	81.814	-4. 54 3	1.00	249.69 249.69
	6338	OD1	ASN E	30	3.012	81.900	-3.481	1.00	249.69
4.5	6339	ND2	ASN E	30	3.030	81.646	-5.721	1.00	249.69
45	6340	Ç	ASN E	30	7.288	81.109	-5.624	1.00	249.69
	6341	0	ASN E	30	7.734	81.191	-6.773	1.00	249.69
	6342 6343	N CA	PHE E	31	8.047	81.290	-4.544	1.00	249.25
	6344	CB	PHE E	31 31	9.464 9.744	81.634	-4.672	1.00	249.25
50	6345	ÇG	PHE	31	8.853	82.979 84.109	-3.973 -4.448	1.00 1.00	249.69
	6346	CD1	PHE E	31	7.546	84.234	-3.971	1.00	249.69 249.69
	6347	CD2	PHE E	31	9.307	85.030	-5.397	1.00	249.69
~	6348	CE1	PHE E	31	6.702	85.255	-4.433	1.00	249.69
	6349	CE2	PHE E	31	8.470	86.054	-5.864	1.00	249.69
55	6350	cz	PHE E	31	7.167	86.166	-5.380	1.00	249.69
	6351	C	PHE E	31	10.439	80.568	-4.166	1.00	249.25
	6352 6353	0 N	PHE E	31	10.399	80.170	-3.004	1.00	249.25
	6354	ČA	PHE E	32 32	11.324 12.329	80.127 79.106	-5.061	1.00	241.74
60	6355	CB	PHE	32	12.131	77.894	-4.757 -5.677	1.00 1.00	241.74 249.69
	6356	CG	PHE E	32	12.858	76.648	-5.224	1.00	249.69
	6357	CD1	PHE E	32	12.489	75.993	-4.048	1.00	249.69
	6358	CD2	PHE E	32	13.905	76.121	-5.984	1.00	249.69
4	6359	CE1	PHE E	32	13.150	74.834	-3.639	1.00	249.69
65	6360	CE2	PHE E	32	14.570	74.962	-5.582	1.00	249.69
	6361	cz	PHE E	32	14.191	74.320	-4.407	1.00	249.69
	6362 6363	C	PHE E	32	13.743	79.667	-4.926 5.400	1.00	241.74
	6364	Ň	GLU E	32 33	13.927 14.739	80.745 78.916	-5.490 -4.465	1.00	241.74
70	6365	ČA	GLU E	33	16.114	79.383	-4.465 -4.531	1.00 1.00	249.60 249.60
-						. 0.000	7.501	1.00	248.00

	6366 6367	CB CG	GLU E	33 .	16.663	79.497	-3.101	1.00	249.49
	6368	CD	GLU E	33 33	17.893 17.724	80.382 81.732	-2.971	1.00	249.49
_	6369	OE1	GLU E	33	16.677	82.386	-3.659 -3.446	1.00 1.00	249.49
5	6370	OE2	GLU E	33	18.641	82.137	-4.409	1.00	249.49 249.49
	6371	C	GLU E	33	17.112	78.603	-5.404	1.00	249.60
	6372 6373	0 N	GLU E VAL E	33	17.820	79.197	-6.225	1.00	249.60
	6374	CA	VAL E	34 34	17.179 18.123	77.285 76.456	-5,229 -5,982	1.00	249.69
10	6375	CB	VAL E	34	18.005	74.970	-5.541	1.00 1.00	249.69 249.69
	6376	CG1	VAL E	34	19.019	74.118	-6.281	1.00	249.69
	6377	CG2	VAL E	34	18.228	74.858	-4.032	1.00	249.69
	6378 6379	C	VAL E VAL E	34	18.014	76.540	-7.511	1.00	249.69
15	6380	Ň	SER E	34 35	16.936 19.152	76.775 76.355	-8.062 -8.178	1.00	249.69
	6381	CA	SER E	35	19.231	76.387	-9.638	1.00 1.00	248.45 248.45
	6382	CB	SER E	35	20.377	77.287	-10.097	1.00	249.69
	6383	og	SER E	35	21.627	76.682	-9.830	1.00	249.69
20	6384 6385	C	SER E SER E	35 35	19.485	74.969	-10.140	1.00	248.45
	6386	Ň.	SER E	35 36	19.572 19.622	74.732 74.036	-11.350 -9.196	1.00	248.45
	6387	CA	SER E	36	19.865	72.628	-9.516	1.00 1.00	249.69 249.69
	6388	CB.	SER E	36	20.966	72.043	-8.614	1.00	244.12
25	6389	og	SER E	36	20.521	71.874	-7.278	1.00	244.12
23	6390 6391	C	SER E SER E	36 36	18.578	71.819	-9.352	1.00	249.69
	6392	. N	THR E	37	18.259 17.836	71.325 71.701	-8.266 -10.449	1.00	249.69
	6393	CA	THR E	37	16.589	70.958	-10.449	1.00 1.00	208.63 208.63
20	6394	CB	THR E	37	15.388	71.911	-10.670	1.00	197.00
30	6395	OG1	THR E	37	15.343	72.880	-9.604	1.00	197.00
	6396 6397	CG2 C	THR E	37	14.089	71.128	-10.693	1.00	197.00
	6398	ŏ	THR E	37 37	16.689 17.186	69. 95 7 70. 277	-11.608 -12.687	1.00	208.63
	6399	Ň	LYS E	38	16.236	68.739	-11.366	1.00 1.00	208.63 223.46
35	6400	CA	LYS E	38	16.309	67.708	-12.384	1.00	223.46
	6401 6402	CB	LYS E	38	16.899	66.425	-11.765	1.00	231.11
	6403	CD	LYS E Lys e	38 38	18. 29 5 18.852	66.620 65.244	-11.158	1.00	231.11
	6404	CE	LYS E	38	20.261	65.344 65.567	-10.528 -9.976	1.00 1.00	231.11
40	6405	NZ	LYS E	38	20.853	64.342	-9.367	1.00	231.11 231.11
	6406	C	LYS E	38	14.947	67.420	-13.018	1.00	223.46
	6407 6408	0	LYS E	38	13.914	67.492	-12.361	1.00	223.46
	6409	N CA	TRP E	39 39	14.951 13.721	67.117	-14.308	1.00	249.08
45	6410	CB	TRP E	39	13.373	66.798 67.909	-15.022 -16.006	1.00 1.00	249.08
	6411	CG	TRP E	39	12.996	69.216	-15.384	1.00	173.34 173.34
	6412	CD2	TRP E	39	11.899	69.476	-14.483	1.00	173.34
	6413 6414	CE2 CE3	TRP E	39	11.857	70.869	-14.267	1.00	173.34
50	6415	CD1	TRP E	39 39	10.957	68.673	-13.840	1.00	173.34
	6416	NE1	TRP E	39	13.550 12.871	70.422 71.424	-15.660 -14.998	1.00 1.00	173.34
	6417	CZ2	TRP E	39	10.911	71.476	-13.440	1.00	173.34 173.34
	6418	CZ3	TRP E	39	10.011	69.281	-13.014	1.00	173.34
55	6419 6420	CH2	TRP E	39	9.995	70.668	-12.828	1.00	173.34
JJ	6421	CO	TRP E	39 39	13.964	65.501	-15.788	1.00	249.08
	6422	Ň	PHE E	40	14.993 13.032	65.363 64.553	-16.450 -15.700	1.00 1.00	249.08
	6423	CA	PHE E	40	13.206	63.281	-16.394	1.00	178.94 178.94
6 0	6424	CB	PHE E	40	13.435	62.145	-15.383	1.00	249.69
60	6425	CG	PHE E	40	14.631	62.341	-14.475	1.00	249.69
	6426 6427	CD1 CD2	PHE E PHE E	40	14.543	63.160	-13.347	1.00	249.69
	6428	CE1	PHE E	40 40	15.836 15.632	61.678 63.313	-14.729 -12.484	1.00	249.69
	6429	CE2	PHE E	40	16.928	61.826	-12.484 -13.873	1.00 1.00	249.69 249.69
65	6430	CZ	PHE E	40	16.824	62.645	-12.748	1.00	249.69
	6431	C	PHE E	40	12.051	62.896	-17.323	1.00	178.94
	6432 6433	0 N	PHE E HIS E	40	11.245	62.027	-16.988	1.00	178.94
	6434	CA	HIS E HIS E	41 41	11.992 10.961	63.534 63.256	-18.488 -19.477	1.00	163.57
70	6435	CB	HIS E	41	11.070	64.259	-19.477 -20.627	1.00 1.00	163.57 157.46
						- T. 100 V		1.00	137.40

	6436 6437	CG CD2	HIS E	41- 41		64.069	-21.695	1.00	157.46
	6438	ND1	HIS E	41	10.104 8.710	64.164 63.777	-23.048	1.00	157.46
_	6439	CE1	HIS E	41	8.018	63.698	-21.411 -22.540	1.00	157.46
5		NE2	HIS E	41	8.840	63.930	-23.544	1.00	157.46
	6441	C	HIS E	41	11.067	61.816	-20.031	1.00 1.00	157.46
	6442 6443	0	HIS E	41	11.955	61.520	-20.841	1.00	163.57 163.57
	6444	N CA	ASN E ASN E	42	10.149	60.937	-19.611	1.00	166.06
10	6445	CB	ASN E	42 42	10.139	59.529	-20.031	1.00	166.06
	6446	CG	ASN E	42	10.165 8.800	59.383 59.655	-21.564	1.00	227.72
	6447	OD1	ASN E	42	8.150	60.654	-22.205	1.00	227.72
	6448	ŊD2	ASN E	42	8.370	58.767	-21.900 -23.101	1.00 1.00	227.72
15	6449	C	ASN E	42	11.348	58.828	-19.424	1.00	227.72
1.5	6450 6451	0 N	ASN E	42	11.820	57.822	-19.950	1.00	166.06 166.06
	6452	CA	GLY E GLY E	43	11.829	59.368	-18.305	1.00	222.62
	6453	č	GLY E	43 43	12.985 14.272	58.804	-17.627	1.00	222.62
•	6454	Ō	GLY E	43	15.139	59.493 59.780	-18.049	1.00	222.62
20	6455	N	SER E	44	14.388	59.764	-17.220 -19.346	1.00	222.62
	6456	CA	SER E	44	15.560	60.424	-19.919	1.00 1.00	232.48
	6457 6458	CB	SER E	44	15.391	60.572	-21.435	1.00	232.48 196.92
	6459	OG C	SER E	44	15.207	59.322	-22.064	1.00	196.92
25	6460	ŏ	SER E SER E	44	15.788	61.806	-19.322	1.00	232.48
	6461	Ň	LEU E	44 45	14,908 16.970	62.661	-19.386	1.00	232.48
	6462	CA	LEU E	45	17.273	62.033 63.331	-18.759	1.00	247.61
	6463	CB	LEU E	45	18.722	63.380	-18.173 -17.682	1.00	247.61
30	6464	CG	LEU E	45	19.128	64.690	-16.996	1.00	238.67
30	6465	CD1	LEU E	45	18.176	64.989	-15.849	1.00 1.00	238.67
	6466 6467	CD2	LEV E	45	20.552	64.584	-16.486	1.00	238.67 238.67
	6468	C	LEU E	45	17.030	64.445	-19.194	1.00	247.61
	6469	Ň	SER E	45 46	17.195 16. 63 0	64.244	-20.401	1.00	247.61
35	6470	CA	SER E	46	16.339	65.616 66.768	-18.700	1.00	233.41
	6471	CB	SER E	46	15.009	67.411	-19.550 -19.131	1.00	233.41
	6472	og	SER E	46	14.644	68.461	-20.012	1.00 1.00	241.98
	6473 6474	C	SER E	46	17.450	67.806	-19.498	1.00	241.98 233.41
40	6475	O N	SER E	46	18.358	67.721	-18.670	1.00	233.41
	6476	CA	GLU E	47	17.353	68.798	-20.378	1.00	249.69
	6477	CB	GLU E	47 47	18.353 18.508	69.858	-20.479	1.00	249.69
	6478	CG	GLU E	47	18.990	70.268 69.136	-21.943	1.00	249.69
45	6479	CD	GLU E	47	19.114	69.555	-22.837 -24.287	1.00	249.69
43	6480	OE1	GLU E	47	18.075	69.901	-24.896	1.00 1.00	249.69 249.69
	6481 6482	OE2 C	GLU E	47	20.247	69.540	-24.819	1.00	249.69
	6483	ŏ	GLU E	47	18.118	71.111	-19.629	1.00	249.69
	6484	Ň	GLU E	47 48	19.014 16.925	71.949	-19.500	1.00	249.69
50	6485	CA	GLU E	48	16.652	71.256 72.417	-19.062	1.00	197.12
	6486	CB	GLU E	48	15.153	72.734	-18.231 -18.213	1.00	197.12
	6487	CG	GLU E	48	14.768	73.878	-17.276	1.00 1.00	231.64 231.64
	6488 6489	CD	GLU E	48	15.355	75.216	-17.688	1.00	231.64
55	6490	OE1 OE2	GLU E	48	14.884	75.786	-18.695	1.00	231.64
	6491	C	GLU E	48 48	16.286	75.698	-17.004	1.00	231.64
	6492	ŏ	GLU E	48	17.147 17.288	72.146	-16.813	1.00	197.12
	6493	N	THR E	49	17.420	70.990 73.221	-16.397	1.00	197.12
60	6494	CA	THR E	49	17.901	73.124	-16.080 -14.707	1.00	219.19
60	6495	CB	THR E	49	19.370	73.557	-14.610	1.00 1.00	219.19
	6496 6497	OG1	THR E	49	19.517	74.871	-15.170	1.00	249.63 249.63
	6498	CG2 C	THR E	49	20.263	72.574	-15.363	1.00	249.63
	6499	ŏ	THR E	49 49	17.060	74.007	-13.794	1.00	219.19
65	6500	Ň	ASN E	49 50	16.949 16.475	73.749	-12.597	1.00	219.19
	6501	CA	ASN E	50	15.625	75.055 75.963	-14.364	1.00	248.24
	6502	CB	ASN E	50	15.070	77.051	-13.603 -14.530	1.00	248.24
	6503 6504	CG	ASN E	50	14.389	78.172	-14.550	1.00 1.00	249.69
70	6505	OD1 ND2	ASN E	50	14.025	78.004	-12.606	1.00	249.69 249.69
- •		NUL	ASN E	50	14.201	79.314	-14.428	1.00	249.69

	6506	С	ASN E	50	14.479	75.129	-13.024	1.00	248.24
	6507	0	ASN E	50	14.117	74.104	-13.598	1.00	248.24
	6508	N :	SER E	51	13.906	75.553	-11.900	1.00	208.41
5	6509	CA .	SER E	51	12.811	74.797	-11.296	1.00	208.41
2	6510	CB	SER E	51	12.509	75.325	-9.894	1.00	181.70
	6511	og	SER E	51	11.848	76.577	-9.948	1.00	181.70
	6512	C	SER E	51	11.524	74.814	-12.142	1.00	208.41
	6513 6514	0	SER E	51	10.625	73.998	-11.929	1.00	208.41
10	6515	N CA	SER E SER E	52	11.434	75.735	-13.100	1.00	201.05
10	6516	CB	SER E SER E	52	10.254	75.830	-13.962	1.00	201.05
	6517	og Og	SER E	52 52	9.717 9.309	77.259	-13.995	1.00	181.26
	6518	č	SER E	52 52	10.551	77.679 75.300	-12.707	1.00	181.26
	6519	ŏ	SER E	52 52	11.180	75.390 76.117	-15.385	1.00	201.05
15	6520	Ň	LEU E	53	10.088	74.194	-16.157 -15.724	1.00	201.05
	6521	CA	LEU E	53	10.287	73.643	-17.058	1.00 1.00	168.60
	6522	СВ	LEU E	53	10.514	72.132	-16.970	1.00	168.60
	6523	CG	LEU E	53	10.304	71.282	-18.231	1.00	122.87 122.87
	6524	CD1	LEU E	53	10.969	71.906	-19.463	1.00	122.87
20	6525	CD2	LEU E	53	10.854	69.900	-17.957	1.00	122.87
	6526	С	LEU E	53	9.077	73.940	-17.340	1.00	168.60
	6527	0	LEU E	53	8.020	73.327	-17.805	1.00	168.60
	6528	N	ASN E	54	9.235	74.892	-18.848	1.00	150.56
25	6529	CA	ASN E	54	. 8.149	75.251	-19.729	1.00	150.56
25	6530	CB	ASN E	54	8.319	76.683	-20.233	1.00	229.83
	6531	CG	ASN E	54	8.080	77.699	-19.151	1.00	229.83
	6532	OD1	ASN E	54	7.052	77.669	-18.479	1.00	229.83
	6533	ND2	ASN E	54	9.029	78.606	-18.972	1.00	229.83
30	6534 6535	C	ASN E	54	8.032	74.311	-20.905	1.00	150.56
50	6536	0 N	ASN E	54	8.977	73.598	-21.260	1.00	150.56
	6537	ČA	ILE E	55 55	6.840	74.322	-21.495	1.00	211.09
	6538	CB	ILE E	55	6.499 5.596	73.504	-22.654	1.00	211.09
	6539	CG2	ILE E	55 55	4.804	72.306 71.809	-22.246	1.00	170.97
35	6540	CG1	ILE E	55	6.460	71.189	-23.445 -21.638	1.00	170.97
	6541	CD1	ILE E	55	5.686	69.960	-21.201	1.00 1.00	170.97
	6542	C	ILE E	55	5.745	74.400	-23.628	1.00	170.97
	6543	. 0	ILE E	55	4.659	74.893	-23.314	1.00	211.09 211.09
	6544	^t N	VAL E	56	6.329	74.624	-24.799	1.00	155.17
40	6545	CA	VAL E	56	5.684	75.466	-25.778	1.00	155.17
	6546	CB	VAL E	56	6.705	76.318	-26.516	1.00	247.89
	6547	CG1	VAL E	56	6.008	77.514	-27.154	1.00	247.89
	6548	CG2	VAL E	56	7.780	76.778	-25.550	1.00	247.89
45	6549	C	VAL E	56	4.917	74.606	-26.770	1.00	155.17
43	6550	0	VAL E	56	4.585	73.468	-26.458	1.00	155.17
	6551 6550	N	ASN E	57	4.639	75.144	-27.959	1.00	169.22
	6552 6553	CA	ASN E	57	3.886	74.432	-28.996	1.00	169.22
	6554	CB	ASN E ASN E	57	4.365	74.837	-30.389	1.00	237.27
50	6555	OD1		57	3.979	76.263	-30.731	1.00	237.27
50	6556	ND2	ASN E ASN E	57 57	2.817	76.650	-30.605	1.00	237.27
	6557	C	ASN E	57 57	4.953	77.055	-31.165	1.00	237.27
	6558	ŏ			3.941	72.925 72.055	-28.825	1.00	169.22
	6559	Ň	ASN E ALA E	57 58	4.860 2.923	72.255 72.424	-29.300	1.00	169.22
55	6560	CA	ALA E	58	2.748	71.015	-28.128 -27.797	1.00	152.74
	6561	СВ	ALA E	58	1.438	70.847	-27.787 -27.040	1.00	152.74
	6562	C	ALA E	58	2.812	70.012	-28.932	1.00 1.00	133.90
	6563	0	ALA E	58	1.888	69.915	-29.751	1.00	152.74 152.74
	6564	N	LYS E	59	3.909	69.258	-28.966	1.00	179.74
60	6565	CA	LYS E	59	4.128	68.226	-29.976	1.00	179.74
	6566	CB	LYS E	59	5.572	68.264	-30.469	1.00	249.69
	6567	CG	LYS E	59	5.967	69.596	-31.093	1.00	249.69
	6568	CD	LYS E	59	7.446	69.638	-31.470	1.00	249.69
65	6569	CE	LYS E	59	7.825	71.010	-32.032	1.00	249.69
65	6570	NZ	LYS E	59	9.265	71.091	-32.425	1.00	249.69
	6571 6570	C	LYS E	59	3.853	66.896	-29.300	1.00	179.74
	6572	0	LYS E	59	4.242	66.677	-28.156	1.00	179.74
	6573 6574	N	PHE E	60	3.175	66.009	-30.009	1.00	187.69
70	6575	CA CB	PHE E	60	2.825	64.706	-29.468	1.00	187.69
	wro	CB	PHE E	60	2.441	63.771	-30.613	1.00	249.39

	6576	CG	PHE E	60	1.209	64.201	-31.352	1.00	249.39
	6577 6570	CD1	PHE E	60	1.035	63.865	-32.689	1.00	249.39
	6578 6579	CD2 CE1	PHE E	60	0.214	64.930	-30.707	1.00	249.39
5	6580	CE2	PHE E	60 60	-0.111 -0.939	64.248 65.319	-33.377	1.00	249.39
•	6581	CZ	PHE E	60	-1.101	64.976	-31.386 -32.724	1.00	249.39
	6582	č	PHE E	60	3.927	64.073	-32.724	1.00 1.00	249.39
	6583	0	PHE E	60	3.642	63.338	-27.683	1.00	187.69 187.69
• •	6584	N	GLU E	61	5.181	64.364	-28.965	1.00	196.09
10	6585	CA	GLU E	61	6.335	63.808	-28.255	1.00	196.09
	6586	CB	GLU E	61	7.623	64.147	-29.010	1.00	249.51
	6587	CG	GLU E	61	7.682	63.618	-30.447	1.00	249.51
	6588 6589	CD OE1	GLU E	61	6.550	64.132	-31.336	1.00	249.51
15	6590	OE2	GLU E GLU E	61	6.341	65.363	-31.403	1.00	249.51
13	6591	C	GLU E	61 61	5.872 6.433	63.302 64.313	-31.976 -26.820	1.00	249.51
	6592	ŏ	GLU E	61	7.042	63.668	-25.965	1.00 1.00	196.09
	6593	Ň	ASP E	62	5.831	65.470	-26.566	1.00	196.09 216.24
	6594	;A	ASP E	62	5.842	66.063	-25.235	1.00	216.24
20	6595	СВ	ASP E	62	5.333	67.500	-25.285	1.00	214.73
	6596	CG	ASP E	62	6.047	68.327	-26.319	1.00	214.73
	6597	OD1	ASP E	62	7.249	68.076	-26.535	1.00	214.73
	6598	OD2	ASP E	62	5.416	69.232	-26.906	1.00	214.73
25	6599 6600	C O	ASP E	62	4.971	65.264	-24.279	1.00	216.24
23	6601	N	ASP E SER E	62 63	5.152	65.325	-23.063	1.00	216.24
	6602	CA	SER E	63	4.009 3.127	64.532 63.707	-24.831	1.00	123.78
	6603	CB	SER E	63	2.085	62.988	-24.015 -24.899	1.00	123.78
	6604	ÖĞ	SER E	63	1.319	63.897	-25.674	1.00 1.00	115.99 115.99
30	6605	C	SER E	63	4.011	62.669	-23.301	1.00	123.78
	6606	0	SER E	63	4.783	61.957	-23.934	1.00	123.78
	6607	N	GLY E	64	3.908	62.584	-21.986	1.00	143.97
	6608	CA	GLY E	64	4.723	61.615	-21.294	1.00	143.97
35	6609 6610	C	GLY E	64	4.739	61.721	-19.786	1.00	143.97
55	6611	0 N	GLY E GLU E	64	3.910	62.406	-19.184	1.00	143.97
	6612	CA CA	GLU E	65 65	5.707 5.904	61.027 60.964	-19.190	1.00	147.25
	6613	CB	GLU E	65	6.138	59.507	-17. 74 3 -17.358	1.00 1.00	147.25
0.2	6614	CG	GLU E	65	6.548	59.268	-15.932	1.00	197.50 197.50
40	6615	CD	GLU E	65	7.152	57.894	-15.759	1.00	197.50
	6616	OE1	GLU E	65	8.198	57.63 0	-16.379	1.00	197.50
	6617	OE2	GLU E	65	6.587	57.076	-15.015	1.00	197.50
	6618	C	GLU E	65	7.097	61.824	-17.309	1.00	147.25
45	6619 6620	0 N	GLU E	65	8.215	61.604	-17.766	1.00	147.25
73	6621	ČA	TYR E TYR E	66 66	6.859	62.792	-16.423	1.00	205.23
	6622	CB	TYR E	66	7.924 7.595	63.682 65.141	-15.948 -16.266	1.00	205.23
	6623	ČĠ	TYR E	66	7.502	65.522	-10.200 -17.726	1.00 1.00	153.79
	6624	CD1	TYR E	66	6.391	65.194	-18.490	1.00	153.79 153.79
50	6625	CE1	TYR E	66	6.265	65.628	-19.806	1.00	153.79
	6626	CD2	TYR E	66	8.491	66.286	-18.316	1.00	153.79
	6627	CE2	TYR E	66	8.377	66.729	-19.628	1.00	153.79
	6628	CZ	TYR E	66	7.265	66.403	-20.368	1.00	153.79
55	6629 6630	ОН	TYR E	66	7.159	66.870	-21.683	1.00	153.79
33	6831	C O	TYR F TYR E	66	8.179	63.597	-14.442	1.00	205.23
	6632	Ň	LYS E	66 67	7.402 9.261	62.979 64.248	-13.710	1.00	205.23
	6633	ĊA	LYS E	67	9.646	64.287	-13.997 -12.580	1.00 1.00	187.13
	6634	CB	LYS E	67	9.961	62.882	-12.360	1.00	187.13 169.14
60	6635	CG	LYS E	67	10.969	62.131	-12.908	1.00	169.14
	6636	CD	LYS E	67	11.160	60.730	-12.365	1.00	169.14
	6637	CE	LYS E	67	11.800	59.810	-13.402	1.00	169.14
	6638	NZ	LYS E	67	12.045	58.414	-12.897	1.00	169.14
65	6639	C	LYS E	67	10.842	65.185	-12.276	1.00	187.13
0,5	6640 6641	O N	LYS E	67 68	11.685	65.433	-13.141	1.00	187.13
	6642	CA	CYS E	68 68	10.902 12.004	65.666 68.515	-11.032	1.00	161.02
	6643	č	CYS E	68	12.590	66.515 66.008	-10.582 -9.267	1.00	161.02
	6644	ŏ	CYS E	68	11.900	65.396	-9.267 -8.456	1.00 1.00	161.02 161.02
70	6645	СВ	CYS E	68	11.567	67.993	-10.447	1.00	132.43
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	6646	SG	CYS E	68	10.402	68.415	-9.105	1.00	132.43
	6647	N	GLN E	69	13.880	66.274	-9.084	1.00	233.39
	6648	CA:	GLN E	69	14.623	65.865	-7.903	1.00	233.39
	6649	CB ·	GLN E	69	15.252	64.494	-8.156	1.00	249.52
5	6650	CG	GLN E	69	16.420	64.156	-7.253	1.00	249.52
	6651	CD	GLN E	69	17.095	62.850	-7.643	1.00	249.52
	6652	OE1	GLN E	69	17.462	62.650	-8.803	1.00	249.52
	6653	NE2	GLN E	69	17.266	61.957	-6.673	1.00	249.52
	6654	С	GLN E	69	15.709	66.900	-7.632	1.00	233.39
10	6655	0	GLN E	69	16.242	67.505	-8.563	1.00	233.39
	6656	N	HIS E	70	16.037	67.108	-6.363	1.00	249.69
	6657	CA	HIS E	70	17.076	68.070	-6.015	1.00	249.69
	6658	CB	HIS E	70	16.657	68.885	-4.790	1.00	243.01
	6659	CG	HIS E	70	15.547	69.852	-5.068	1.00	243.01
15	6660	CD2	HIS E	70	14.356	70.039	-4.454	1.00	243.01
	6661	ND1	HIS E	70	15.605	70.774	-6.089	1.00	243.01
	6662	CE1	HIS E	70	14.495	71.493	-6.096	1.00	243.01
	6663	NE2	HIS E	70	13.721	71.068	-5.114	1.00	243.01
20	6664	Č	HIS E	70	18.414	67.388	-5.761	1.00	249.69
20	6665	0	HIS E	70	18.575	66.198	-6.034	1.00	249.69
	6666	N	GLN E	71	19.370	68.148	-5.238	1.00	231.62
	6667	CA	GLN E	71	20.708	67.634	-4.952	1.00	231.62
	6668	CB	GLN E	71	21.554	68.756	-4.329	1.00	249.69
25	6669	CG	GLN E	71	23.080	68.559	-4.380	1.00	249.69
23	6670	CD	GLN E	71	23.634	68.488	-5.803	1.00	249.69
	6671	OE1	GLN E	71	23.304	69.316	·6.663	1.00	249.69
	6672	NE2	GLN E	71	24.495	67.503	-6.049	1.00	249.69
	6673	C	GLN E	71	20.677	66.413	-4.022	1.00	231.62
30	6674	0	GLN E	71	21.311	65.389	-4.298	1.00	231.62
50	6675 6676	N CA	GLN E	72	19.928	66.528	-2.928	1.00	249.69
	6677	CA CB	GLN E	72	19.819	65.448	-1.951	1.00	249.69
	6678	CG	GLN E	72	20.601	65.834	-0.689	1.00	249.69
	6679	CD	GLN E GLN E	72	20.626	64.791	0.419	1.00	249.69
35	6680	OE1	GLN E GLN E	72	21.284	65.315	1.687	1.00	249.69
33	6681	NE2	GLN E	72 70	22.439	65.746	1.664	1.00	249.69
	6682	C	GLN E	72	20.549	65.281	2.799	1.00	249.69
	6683	ŏ	GLN E	72 72	18.349	65.170	-1.607	1.00	249.69
	6684	Ň	VAL E	73	17.948	65.208	-0.444	1.00	249.69
40	6685	CA	VAL E	73 73	17.544 16.128	64.899 64.614	-2.627	1.00	249.30
	6686	CB	VAL E	73	15.243	65.860	-2.427 -2.707	1.00	249.30
	6687	CG1	VAL E	73	13.838	65.814	-2.707 -2.192	1.00 1.00	249.69
	6688	CG2	VAL E	73	15.843	67.101	-2.058	1.00	249.69
	6689	C	VAL E	73	15.709	63.512	-3.386	1.00	249.69
45	6690	0	VAL E	73	16.183	63.451	-4.516	1.00	249.30 249.30
	6691	N	ASN E	74	14.817	62.642	-2.937	1.00	249.46
	6692	CA	ASN E	74	14.345	61.555	-3.783	1.00	249.46
	6693	CB	ASN E	74	13.714	60.460	-2.912	1.00	249.69
	6694	CG	ASN E	74	14.665	59.960	-1.825	1.00	249.69
50	6695	OD1	ASN E	74	15.859	59.769	-2.080	1.00	249.69
	6696	ND2	ASN E	74	14.139	59.737	-0.621	1.00	249.69
	6697	С	ASN E	74	13.346	62.081	-4.826	1.00	249.46
	6698	0	ASN E	74	12.387	62.774	-4.485	1.00	249.46
	6699	N	GLU E	75	13.587	61.755	-6.094	1.00	249.69
55	6700	CA	GLU E	75	12.740	62.194	-7.209	1.00	249.69
	6701	CB	GLU E	7 5	13.082	61.386	-8.468	1.00	249.69
	6702	ÇG	GLU E	75	13.431	59.924	-8.199	1.00	249.69
	6703	CD	GLU E	75	14.002	59.221	-9.425	1.00	249.69
60	6704	OE1	GLU E	75	14.946	59.768	-10.042	1.00	249.69
60	6705	OE2	GLU E	75	13.515	58.118	-9.768	1.00	249.69
	6706	Ç	GLU E	75	11.233	62.147	-6.941	1.00	249.69
	6707	0	GLU E	75	10.724	61.213	-6.320	1.00	249.69
	6708	N	SER E	76	10.531	63.168	-7.428	1.00	190.25
65	6709	CA	SER E	76	9.083	63.302	-7.244	1.00	190.25
O)	6710	CB	SER E	76	8.613	64.671	-7.743	1.00	199.25
	6711	og .	SER E	76	8.614	64.717	-9.163	1.00	199.25
	6712	C	SER E	76	8.265	62.236	-7.954	1.00	190.25
	6713	0	SER E	76	8.728	61.612	-8.907	1.00	190.25
70	6714 6715	N CA	GLU E	77	7.038	62.044	-7.481	1.00	235.50
, 0	0713	CA	GLU E	77	6.135	61.072	-8.079	1.00	235.50

	6716	СВ	GLU E	77 ·	4.839	60.973	-7.269	1.00	249.14
	6717	CG	GLU E	77	5.029	60.405	-5.870	1.00	249.14
	6718	CD:	GLU E	77	5.532	58.966	-5.879	1.00	249.14
5	6719	OE1.	GLU E	77	5.869	58.450	-6.966	1.00	249.14
)	6720	OE2	GLU E	77	5.594	58.349	-4.795	1.00	249.14
	6721 6722	C	GLU E GLU E	77	5.826	61.543	-9.488	1.00	235.50
	6723	N	PRO E	77 78	5.181	62.569	-9.672	1.00	235.50
	6724	CD	PRO E	78 78	6.280 6.805	60.791 59.420	-10.505	1.00	173.10
10	6725	CA	PRO E	78	6.055		-10.383	1.00	109.00
	6726	CB	PRO E	78	6.320	61.144 59.831	-11.915 -12.652	1.00	173.10
	6727	CG	PRO E	78	7.324	59.145	-12.652	1.00	109.00
	6728	c	PRO E	78	4.648	61.657	-12.182	1.00	109.00
	6729	ŏ	PRO E	78	3.721	61.375	-11.410	1.00	173.10
15	6730	Ň	VAL E	79	4.490	62.430	-13.253	1.00	173.10 170.14
	6731	CA	VAL E	79	3.168	62.929	-13.628	1.00	170.14
	6732	CB	VAL E	79	2.986	64.448	-13.378	1.00	117.67
	6733	CG1	VAL E	79	1.708	64.936	-14.057	1.00	117.67
20	6734	CG2	VAL E	79	2.879	64.719	-11.889	1.00	117.67
20	6735	Ç	VAL E	79	3.081	62.669	-15.111	1.00	170.14
	6736	0	VAL E	79	4.093	62.798	-15.803	1.00	170.14
	6737	N	TYR E	80	1.903	62.292	-15.605	1.00	121.68
	6738	CA	TYR E	80	1.782	62.023	-17.028	1.00	121.68
25	6739	CB	TYR E	80	1.072	60.700	-17.272	1.00	162.42
25	6740 6741	CG CD1	TYR E	80	1.291	60.179	-18.675	1.00	162.42
	6742	CE1	TYR E TYR E	80 80	2.439	59.447	-18.995	1.00	162.42
	6743	CD2	TYR E	80	2.661 0.370	58.981	-20.301	1.00	162.42
	6744	CE2	TYR E	80	0.588	60.437 59.980	-19.696	1.00	162.42
30	6745	CZ	TYR E	80	1.732	59.256	-21.002 -21.290	1.00	162.42
	6746	OH	TYR E	80	1.960	58.803	-21.290 -22.557	1.00 1.00	162.42 162.42
	6747	Ċ	TYR E	80	1.040	63.132	-17.752	1.00	121.68
	6748	Ō	TYR E	80	0.022	63.642	-17.277	1.00	121.68
	6749	N	LEU E	81	1.562	63.511	-18.906	1.00	108.83
35	6750	CA	LEU E	81	0.943	64.545	-19.706	1.00	108.83
	6751	CB	LEU E	81	1.930	65.677	-19.978	1.00	110.26
	6752	CG	LEU E	81	1.380	66.724	-20.946	1.00	110.26
	6753	CD1	LEV E	81	0.173	67.390	-20.296	1.00	110.26
40	6754	CD2	LEU E	81	2.432	67.748	-21.292	1.00	110.26
40	6755	C	LEU E	81	0.514	63.944	-21.028	1.00	108.83
	6756	0	LEU E	81	1.308	63.312	-21.701	1.00	108.83
	6757	N OA	GLU E	82	-0.740	64.132	-21.407	1.00	99.21
	6758 6759	CA CB	GLU E	82	-1.194	63.601	-22.679	1.00	99.21
45	6760	CG	GLU E	82 82 ·	-2.359 -2.479	62.625	-22.473	1.00	224.57
45	6761	CD	GLU E	82	-2.479 -3.618	61.592 60.615	-23.590	1.00	224.57
	6762	OE1	GLU E	82	-3.903	60.282	-23.373	1.00	224.57
	6763	OE2	GLU E	82	-4.216	60.166	-22.198 -24.380	1.00 1.00	224.57
	6764	č	GLU E	82	-1.623	64.749	-23.596	1.00	224.57 99.21
50	6765	ŏ	GLU E	82	-2.287	65.700	-23.142	1.00	99.21
	6766	N	VAL E	83	-1.231	64.670	-24.876	1.00	128.82
	6767	CA	VAL E	83	-1.599	65.690	-25.871	1.00	128.82
	6768	CB	VAL E	83	-0.388	66.250	-26.586	1.00	97.06
	6769	CG1	VAL E	83	-0.835	67.323	-27.572	1.00	97.06
55	6770	CG2	VAL E	83	0.585	66.824	-25.562	1.00	97.06
	6771	Ç	VAL E	83	-2.564	65.129	-26.915	1.00	128.82
	6772	0	VAL E	83	-2.424	63.998	-27.378	1.00	128.82
	6773	N	PHE E	84	-3.528	65.951	-27.302	1.00	126.16
60	6774	CA	PHE E	84	-4.572	65.524	-28.218	1.00	126.16
00	6775	CB	PHE E	84	-5.893	65.416	-27.473	1.00	129.94
	6776 6777	CG CD1	PHE E	84	-5.885	64.434	-26.357	1.00	129.94
	6778	CD1 CD2	PHE E PHE E	84	-5.361	64.755	-25.107	1.00	129.94
	6779	CE1	PHE E	84 84	-6.432 -5.372	63.191	-26.547	1.00	129.94
65	6780	CE2	PHE E	84 84	-5.372 -6.449	63.832 63.832	-24.070	1.00	129.94
	6781	CZ	PHE E	84	-5.924	62.262 62.585	-25.522 -24.279	1.00	129.94
	6782	Č	PHE E	84	-4.872	66.377	-24.278 -29.422	1.00	129.94
	6783	ŏ	PHE E	84	-4.588	67.571	-29.422 -29.466	1.00 1.00	126.16
	6784	N	SER E	85	-5.510	65.732	-30.385	1.00	126.16 167.68
70	6785	CA	SER E	85	-5.960	66.381	-31.604	1.00	167.68

	6786	СВ	SER E	85	-5.136	65.957	-32.815	1.00	221.67
	6787	og .	SER E	85	-5.627	66.593	-33.981	1.00	221.67
	6788	C .	SER E	85	-7.390	65.909	-31.783	1.00	167.68
5	6789 6790	O N	SER E ASP E	85 86	-7.620 -8.342	64.718 66.840	-32.008	1.00	167.68
_	6791	CA	ASP E	86	-9.766	66.530	-31.661 -31.793	1.00 1.00	124.68
	6792	CB	ASP E	86	-10.199	65.550	-30.697	1.00	124.68 146.90
	6793	CG	ASP E	86	-11.214	64.542	-31.189	1.00	146.90
	6794	OD1	ASP E	86	-12.235	64.955	-31.792	1.00	146.90
10	6795	OD2	ASP E	86	-10.979	63.329	-30.978	1.00	146.90
	6796	C	ASP E	86	-10.583	67.792	-31.658	1.00	124.68
	6797	0	ASP E	86	-10.064	68.815	-31.244	1.00	124.68
	6798 6799	N CA	TRP E	87 87	-11.864	67.722	-31.995	1.00	145.58
15	6800	CB	TRP E	87 87	-12.717 -14.072	68.901 68.644	-31.880 -32.537	1.00	145.58
••	6801	CG	TRP E	87	-14.072	69.003	-32.537	1.00 1.00	249.10
	6802	CD2	TRP E	87	-13.811	68.127	-35.085	1.00	249.10 249.10
	6803	CE2	TRP E	87	-13.877	68.898	-36.268	1.00	249.10
••	6804	CE3	TRP E	87	-13.517	⊸ ∂.759	-35.187	1.00	249.10
20	6805	CD1	TRP E	87	-14.291	70.241	-34.532	1.00	249.10
	6806	NE1	TRP E	87	-14.173	70.189	-35.899	1.00	249.10
	6807	CZ2	TRP E	87	-13.663	68.354	-37. 538	1.00	249.10
	6808 6809	CZ3 CH2	TRP E	87	-13.302	66.212	-36.451	1.00	249.10
25	6810	C	TRP E	87 87	-13.379 -12.890	67.011	-37.610	1.00	249.10
23	6811	ŏ	TRP E	87 87	-12.890 -12.607	69.314 70.467	-30.433	1.00	145.58
	6812	Ň	LEU E	88	-13.345	68.377	-30.077 -29.605	1.00 1.00	145.58
	6813	CA	LEU E	88	-13.521	68.658	-28.190	1.00	109.18 109.18
	6814	CB	LEU E	88	-15.001	68.601	-27.819	1.00	123.07
30	6815	CG	LEU E	88	-15.885	69.659	-28.476	1.00	123.07
	6816	CD1	LEU E	88	-17.294	69.581	-27.913	1.00	123.07
	6817	CD2	LEU E	88	-15.326	71.049	-28.223	1.00	123.07
	6818	C	LEU E	88	-12.715	67.699	-27.298	1.00	109.18
35	6819 6820	O N	LEU E	88	-12.590	66.501	-27.598	1.00	109.18
55	6821	CA	LEU E	89 89	-12.147 -11.380	68.231 67.420	-26.214 -25.270	1.00	123.09
	6822	CB	LEU E	89	-9.891	67.745	-25.270 -25.358	1.00 1.00	123.09 138.74
	6823	CG	LEU E	89	-9.031	66.974	-24.347	1.00	138.74
40	6824	CD1	LEU E	89	-9.313	65.467	-24.460	1.00	138.74
40	6825	CD2	LEU E	89	-7.565	67.265	-24.589	1.00	138.74
	6826	C	LEU E	89	-11.865	67.724	-23.864	1.00	123.09
	6827	0	LEU E	89	-11.959	68.879	-23.478	1.00	123.09
	6828 6829	N CA	LEV E	90	-12.184	66.695	-23.097	1.00	99.50
45	6830	CB	LEU E	90 90	-12.659 -13.556	66.912 65.759	-21.737	1.00	99.50
	6831	CG	LEU E	90	-13.932	65.784	-21.305 -19.817	1.00 1.00	113.63 113.63
	6832	CD1	LEU E	90	-14.685	67.054	-19.527	1.00	113.63
	6833	CD2	LEU E	90	-14.770	64.565	-19.457	1.00	113.63
	6834	С	LEU E	90	-11.502	67.023	-20.773	1.00	99.50
50	6835	0	LEU E	90	-10.779	66.046	-20.570	1.00	99.50
	6836	N	GLN E	91	-11.316	68.194	-20.170	1.00	92.89
	6837 6838	CA	GLN E	91	-10.202	68.367	-19.228	1.00	92.89
	6839	CB CG	GLN E	91 01	-9.505	69.690	-19.467	1.00	161,25
55	6840	CD	GLN E	91 91	-8.933 -8.254	69.836 71.177	-20.848 -21.039	1.00	161.25
	6841	OE1	GLN E	91	-8.877	72.232	-20.866	1.00 1.00	161.25
	6842	NE2	GLN E	91	-6.968	71.149	-21.398	1.00	161.25 161.25
	6843	С	GLN E	91	-10.632	68.289	-17.770	1.00	92.89
60	6844	0	GLN E	91	-11.680	68.833	-17.391	1.00	92.89
60	6845	N	ALA E	92	-9.814	67.612	-16.961	1.00	113.22
	6846	CA	ALA E	92	-10.114	67.458	-15.544	1.00	113.22
	6847 6848	CB C	ALA E ALA E	92	-10.393	65.997	-15.212	1.00	187.04
	6849	ŏ	ALA E	92 92	-8.942 -7.777	67.975 67.803	-14.720	1.00	113.22
65	6850	Ň	SER E	93	-7.777 -9.271	67.802 68.623	-15.105 -13.506	1.00	113.22
-	6851	ĊA	SER E	93	-8.279	69.178	-13.596 -12.676	1.00 1.00	114.34
	6852	CB	SER E	93	-8.973	69.762	-11.425	1.00	114.34 137.73
	6853	OG	SER E	93	-9.879	68.858	-10.813	1.00	137.73
70	6854	C	SER E	93	-7.326	68.043	-12.300	1.00	114.34
70	6855	0	SER E	93	-6.140	68.078	-12.593	1.00	114.34

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	6856	N	ALA E	94	-7.869	67.028	-11.653	1.00	121.13
	6857	CA	ALA E	94	-7.113	65.858	-11.255	1.00	121.13
	6858	CB:	ALA E	94	-6.898	65.855	-9.748	1.00	206.55
5	6859	Ċ.	ALA E	94	-8.008	64.684	-11.671	1.00	121.13
J	6860	0	ALA E	94	-9.235	64.832	-11.768	1.00	121.13
	6861 6862	N CA	GLU E GLU E	95	-7.424	63.520	-11.937	1.00	135.32
	6863	CB	GLU E	95 05	-8.238	62.378	-12.347	1.00	135.32
	6864	CG	GLU E	95 95	-7.496 -7.262	61.564	-13.390	1.00	189.07
10	6865	CD.	GLU E	95	-7.262 -6.736	62.342 61.482	-14.660 -15.780	1.00	189.07
	6866	OE1	GLU E	95	-6.466	62.025	-16.876	1.00	189.07
	6867	OE2	GLU E	95	-6.596	60.259	-15.563	1.00 1.00	189.07
	6868	c	GLU E	95	-8.632	61.500	-11.171	1.00	189.07
	6869	0	GLU E	95	-9.632	60.772	-11.247	1.00	135.32 135.32
15	6870	N	VAL E	96	-7.854	61.581	-10.085	1.00	121.52
	6871	CA	VAL E	96	-B.118	60.807	-8.865	1.00	121.52
	6872	СВ	VAL E	96	-6.994	59.808	-8.591	1.00	138.26
	6873	<u>1</u> 90	VAL E	96	-7.480	58.754	-7.615	1.00	138.26
20	6874	ÇG2	VAL E	96	-6.534	59.178	-9.895	1.00	138.26
20	6875	C	VAL E	96	-8.237	61.741	-7.664	1.00	121.52
	6876 6877	0	VAL E	96	-7.376	62.598	-7.462	1.00	121.52
	6878	N CA	VAL E VAL E	97	-9.278	61.566	-6.854	1.00	165.05
	6879	CB	VAL E VAL E	97 97	-9.458	62.462	-5.725	1.00	165.05
25	6880	CG1	VAL E	97	-10.499 -10.338	63.511 64.666	-6.048	1.00	119.89
45	6881	CG2	VAL E	97	-10.338	63.961	-5.113 7.400	1.00	119.89
	6882	Č	VAL E	97	-9.856	61.866	-7.482 -4.380	1.00	119.89
	6883	ŏ	VAL E	97	-10.545	60.844	-4.325	1.00 1.00	165.05
	6884	N	MET E	98	-9.427	62.544	-3.306	1.00	165.05 159.57
30	6885	CA	MET E	98	-9.713	62.161	-1.914	1.00	159.57
	6886	CB	MET E	98	-8.657	62.750	-0.973	1.00	249.69
	6887	CG	MET E	98	-7.247	62.228	-1.152	1.00	249.69
	6888	SD	MET E	98	-7.038	60.577	-0.463	1.00	249.69
25	6889	CE	MET E	98	-6.946	60.948	1.288	1.00	249.69
35	6890	C	MET E	98	-11.071	62.740	-1.522	1.00	159.57
	6891	0	MET E	98	-11.268	63.954	-1.606	1.00	159.57
	6892 6893	N CA	GLU E GLU E	99	-11.993	61.888	-1.075	1.00	145.00
	6894	CB	GLU E GLU E	99 99	-13.327 -13.989	62.349	-0.683	1.00	145.00
40	6895	ČG	GLU E	99	-15.505	61.342 61.399	0.261	1.00	208.72
	6896	CD	GLU E	99	-16.126	60.618	0.247 1.385	1.00 1.00	208.72
	6897	OE1	GLU E	99	-15.593	59. 542	1.731	1.00	208.72
	6898	OE2	GLU E	99	-17.154	61.079	1.923	1.00	208.72 208.72
	6899	С	GLU E	99	-13.241	63.699	0.022	1.00	145.00
45	6900	0	GLU E	99	-12.518	63.854	0.993	1.00	145.00
	6901	N	GLY E	100	-13.970	64.686	-0.473	1.00	140.46
	6902	CA	GLY E	100	-13.941	65.989	0.164	1.00	140.46
	6903	C	GLY E	100	-13.192	67.07 0	-0.585	1.00	140.46
50	6904	0	GLY E	100	-13.449	68.256	-0.353	1.00	140.46
50	6905 6906	N CA	GLN E GLN E	101	-12.279	66.679	-1.475	1.00	158.90
	6907	CB	GLN E	101	-11.493	67.641	-2.259	1.00	158.90
	6908	CG	~	101	-10.255	66.969	-2.835	1.00	248.74
	6909	CD	GLN E	101 101	-9.216 -9.002	66. 62 5 67. 76 4	-1.80	1.00	248.74
55	6910	OE1	GLN E	101	-9.873	68.070	-0.831	1.00	248.74
	6911	NE2	GLN E	101	-7.848	68.409	-0.017 -0.919	1.00	248.74
	6912	C	GLN E	101	-12.290	68.324	-3.371	1.00	248.74
	6913	Ö	GLN E	101	-13.445	67.987	-3.628	1.00 1.00	158.90 158.90
	6914	N	PRO E	102	-11.657	69.302	-4.050	1.00	164.28
60	6915	CD	PRO E	102	-10.406	69.971	-3.720	1.00	154.28
	6916	CA	PRO E	102	-12.358	69.987	-5.140	1.00	164.28
	6917	СВ	PRO E	102	-11.739	71.379	-5.074	1.00	154.28
	6918	CG	PRO E	102	-10.312	71.040	-4.796	1.00	154.28
65	6919	C	PRO E	102	-12.161	69.327	-6.496	1.00	164.28
UJ	6920	0	PRO E	102	-11.119	68.720	-6.771	1.00	164.28
	6921	N	LEU E	103	-13.169	69.467	-7.358	1.00	176.34
	6922 6923	CA CB	LEU E	103	-13.127	68.873	-8.679	1.00	176.34
	6924	CG	LEV E	103	-13.983	67.617	-8.690	1.00	122.49
70	6925	CD1	LEU E	103 103	-13.722 -12.310	66.849	-9. 9 71	1.00	122.49
. 🕶			E	103	-12.310	66.308	-9.883	1.00	122.49

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	6926	CD2	LEU E	103	-14.724	65.736	-10.156	1.00	122.49
	6927	C .	LEU E	103	-13.618	69.805	<i>-</i> 9.776	1.00	176.34
	6928 6929	0 :. N	LEU E	103	-14.736	70.305	-9.696	1.00	176.34
5	6930	CA	PHE E	104 104	-12.805	70.027	-10.806	1.00	126.68
J	6931	CB	PHE E	104	-13.233 -12.412	70.890 72.174	-11.903	1.00	126.68
	6932	CG	PHE E	104	-12.412	72.174 72.934	-11.954 -10.681	1.00	239.90
	6933	CD1	PHE E	104	-11.612	72.520	-9.623	1.00 1.00	239.90
	6934	CD2	PHE E	104	-13.201	74.060	-10.528	1.00	239.90
10	6935	CE1	PHE E	104	-11.608	73.221	-8.416	1.00	239.90 239.90
	6936	CE2	PHE E	104	-13.211	74.770	-9.331	1.00	239.90
	6937	CZ	PHE E	104	-12.410	74.349	-8.269	1.00	239.90
	6938	C	PHE E	104	-13.110	70.197	-13.250	1.00	126.68
15	6939 6940	0 N	PHE E	104	-12.033	69.723	-13.600	1.00	126.68
13	6941	CA	LEU E	105 105	-14.208 -14.176	70.136	-14.003	1.00	132.08
	6942	CB	LEU E	105	-15.249	69.524 68.452	-15.327	1.00	132.08
	6943	CG	LEU E	105	-15.131	67.347	-15.456 -14.414	1.00 1.00	106.14
	6944	CD1	LEU E	105	-16.174	66.283	-14.719	1.00	106.14 106.14
20	6945	CD2	LEU E	105	-13.704	66.777	-14.429	1.00	106.14
	6946	Ç	LEU E	105	-14.413	70.618	-16.344	1.00	132.08
	6947	0	LEU E	105	-15.119	71.592	-16.064	1.00	132.08
	6948 6949	N CA	ARG E	106	-13.848	70.456	-17.532	1.00	113.14
25	6950	CA CB	ARG E ARG E	106	-13.996	71.486	-18.543	1.00	113.14
25	6951	CG	ARG E	106 106	-12.753 -12.740	72.363	-18.492	1.00	157.66
	6952	CD	ARG E	106	-12.740	73.498 74.197	-19.454 -19.428	1.00	157.66
	6953	NE	ARG E	106	-11.356	75.192	-20.478	1,00 1.00	157.66
	6954	CZ	ARG E	106	-10.256	75.566	-21.103	1.00	157.66 157.66
30	6955	NH1	ARG E	106	-9.094	75.020	-20.774	1.00	157.66
	6956	NH2	ARG E	106	-10.331	76.473	-22.071	1.00	157.66
	6957	C	ARG E	106	-14.172	70.905	-19.932	1.00	113.14
	6958 6959	0 N	ARG E CYS E	106	-13.363	70.068	-20.365	1.00	113.14
35	6960	ČA	CYS E	107 107	-15.235 -15.456	71.312	-20.620	1.00	132.92
	6961	č`	CYS E	107	-14.646	70.829 71.786	-21.979 -22.808	1.00	132.92
	6962	ō	CYS E	107	-15.068	72.922	-22.996	1.00 1.00	132.92 132.92
	6963	CB	CYS E	107	-16.923	70.942	-22.370	1.00	146.71
40	6964	SG	CYS E	107	-17.372	70.056	-23.927	1.00	146.71
40	6965	N	HIS E	108	-13.483	71.339	-23.282	1.00	154.76
	6966	CA	HIS E	108	-12.576	72.195	-24.052	1.00	154.76
	6967 6968	CB CG	HIS E	108	-11.130	71.911	-23.639	1.00	172.76
	6969	CD2	HIS E HIS E	108 108	-10.136 -8.957	72.910 72.738	-24.161	1.00	172.76
45	6970	ND1	HIS E	108	-10.277	74.262	-24.810	1.00	172.76
	6971	CE1	HIS E	108	-9.221	74.888	-23.967 -24.473	1.00 1.00	172.76
	6972	NE2	HIS E	108	-8.409	73.987	-24.986	1.00	172.76 172.76
	6973	C	HIS E	108	-12.688	72.087	-25.560	1.00	154.76
50	6974	0	HIS E	108	-12.576	70.997	-26.129	1.00	154.76
30	6975	N	GLY E	109	-12.892	73.240	-26.194	1.00	128.76
	69 7 6 6977	CA C	GLY E GLY E	109	-13.007	73.287	-27.637	1.00	128.76
	6978	ŏ	GLY E	109 109	-11.632 -10.666	73.334	-28.260	1.00	128.76
	6979	Ň	TRP E	110	-11.539	73.574 73.092	-27.552	1.00	128.76
55	6980	CA	TRP E	110	-10.260	73.136	-29.566 -30.251	1.00	154.27
	6981	CB	TRP E	110	-10.312	72.268	-31.503	1.00 1.00	154.27 170.55
	6982	CG	TRP E	110	-9.107	72.411	-32.397	1.00	170.55
	6983	CD2	TRP E	110	-7.963	71.539	-32.468	1.00	170.55
60	6984	CE2	TRP E	110	-7.073	72.098	-33,406	1.00	170.55
60	6985 6986	CE3 CD1	TRP E	110	-7.606	70.345	-31.825	1.00	170.55
	6987	NE1	TRP E	110 110	-8.8 63	73.422	-33.270	1.00	170.55
	6988	CZ2	TRP E	110	-7.645 -5.840	73.242 71.501	-33.877	1.00	170.55
	6989	CZ3	TRP E	110	-6.37 5	69.755	-33.719 -32.137	1.00	170.55
65	6990	CH2	TRP E	110	-5.509	70.339	-32.137 -33.077	1.00 1.00	170.55 170. 5 5
	6991	С	TRP E	110	-9.897	74.586	-30.600	1.00	170.55
	6992	0	TRP E	110	-10.786	75.431	-30.767	1.00	154.27
	6993	N	ARG E	111	-8.596	74.878	-30.693	1.00	180.74
70	6994 6995	CA CB	ARG E	111	-8.116	76.229	-30.994	1.00	180.74
, 5	U##3	06	ARG E	111	-8.361	76.580	-32.460	1.00	249.46

	6996 6997 6998	CG CD NE:	ARG E ARG E ARG E	111 111 111	-7.220 -7.366	76.198 76.870	-33.381 -34.738	1.00	249.46 249.46
5	6999 7000	CZ NH1	ARG E	111 111	-6.076 -5.295 -5.672	77.324 78.200 78.720	-35.248 -34.623 -33.463	1.00 1.00 1.00	249.46 249.46 249.46
	7001 7002 7003	NH2 C O	ARG E ARG E ARG E	111 111 111	-4.136 -8.804 -9.013	78.557 77.263 78.408	-35.155 -30.104 -30.490	1.00 1.00 1.00	249.46 180.74 180.74
10	7004 7005 7006	N CA CB	ASN E ASN E ASN E	112 112 112	-9.156 -9.815 -8.820	76.839 77.702 78.719	-28.903 -27.949 -27.388	1.00 1.00 1.00	179.60 179.60 235.58
	7007 7008 7009	CG OD1 ND2	ASN E ASN E ASN E	112 112 112	-9.314 -10.493 -8.413	79.373 79.276 80.052	-26.110 -25.757 -25.412	1.00 1.00	235.58 235.58
15	7010 7011 7012	C O N	ASN E ASN E TRP E	112 112	-11.002 -11.299	78.426 79.551	-28.579 -28.193	1.00 1.00 1.00	235.58 179.60 179.60
20	7013 7014	CA CB	TRP E	113 113 113	-11.671 -12.841 -13.343	77.798 78.420 77.633	-29.550 -30.174 -31.368	1.00 1.00 1.00	181.35 181.35 198.74
20	7015 7016 7017	CG CD2 CE2	TRP E TRP E	113 113 113	-12.618 -12.345 -11.666	77.902 76.965 77.674	-32.604 -33.651 -34.676	1.00 1.00 1.00	198.74 198.74 198.74
25	7018 7019 7020	CE3 CD1 NE1	TRP E TRP E TRP E	113 113 113	-12.603 -12.114 -11.527	75.599 79.099 78.973	-33.823 -33.018 -34.267	1.00 1.00 1.00	198.74 198.74 198.74
	7021 7022 7023	CZ2 CZ3 CH2	TRP E TRP E TRP E	113 113 113	-11.246 -12.185 -11.515	77.052 74.983 75.711	-35.861 -34.994 -36.001	1.00 1.00 1.00	198.74 198.74 198.74
30	7024 7025 7026	C O N	TRP E TRP E ASP E	113 113 114	-13.968 -13.763 -15.168	78.478 78.229 78.806	-29.164 -27.974 -29.629	1.00 1.00 1.00	181.35 181.35 198.96
	7027 7028 7029	CA CB CG	ASP E ASP E	114 114 114	-16.312 -17.015 -16.337	78.881 80.250 81.350	-28.724 -28.852 -28.026	1.00 1.00 1.00	198.96 241.05
35	7030 7031 7032	OD1 OD2 C	ASP E ASP E ASP E	114 114 114	-16.217 -15.928 -17.299	81.193 82.374 77.746	-26.790 -28.614	1.00 1.00	241.05 241.05 241.05
40	7033 7034 7035	O N CA	ASP E VAL E VAL E	114 115	-17.646 -17.732	77.470 77.083	-28.994 -30.151 -27.922	1.00 1.00 1.00	198.96 198.96 162.46
10	7036 7037 7038	CB CG1	VAL E	115 115 115	-18.686 -18.191 -19.018	75.985 74.726 73.528	-28.039 -27.316 -27.751	1.00 1.00 1.00	162.46 122.72 122.72
45	7039 70 40	CG2 C O	VAL E VAL E	115 115 115	-16.727 -20.033 -20.084	74.493 76.382 77.042	-27.603 -27.434 -26.385	1.00 1.00 1.00	122.72 162.46 162.46
	7041 7042 7043	N CA CB	TYR E TYR E TYR E	116 116 116	-21.114 -22.468 -23.177	75.972 76.285 77.143	-28.096 -27.648 -28.693	1.00 1.00 1.00	116.01 116.01 231.08
50	7044 7045 7046	CG CD1 CE1	TYR E TYR E TYR E	116 116 116	-22.540 -21.643 -21.024	78.498 78.743 79.992	-28.877 -29.918 -30.062	1.00 1.00 1.00	231.08 231.08 231.08
EE	7047 7048 7049	CD2 CE2 CZ	TYR E TYR E TYR E	116 116 116	-22.805 -22.194 -21.306	79.531 80.780 81.006	-27.984 -28.114 -29.154	1.00 1.00 1.00	231.08 231.08 231.08
55	7050 7051 7052	OH C O	TYP E TYR E TYR E	116 116 116	-20.705 -23.279 -22.829	82.241 75.007 73.909	-29.278 -27.387 -27. 72 2	1.00 1.00 1.00	231.08 116.31 116.01
60	7053 7054 7055	N CA CB	LYS E LYS E LYS E	117 117 117	-24.472 -25.359 -26.062	75.163 74.042 73.531	-26.792 -26.454 -27.701	1.00 1.00 1.00	118.22 118.22 223.92
	7056 7057 7058	CG CD CE	LYS E LYS E LYS E	117 117 117	-27.319 -28.221 -28.639	74.305 73.481 72.150	-28.079 -29.013 -28.354	1.00 1.00	223.92 223.92
65	7059 7060 7061	NZ C O	LYS E LYS E LYS E	117 117 117	-29.508 -24.619	71.267 72.877	-29.203 -25.764	1.00 1.00 1.00	223.92 223.92 118.22
	7062 7063 7064	N CA CB	VAL E VAL E	118 118	-24.736 -23.883 -23.120	71.712 73.200 72.205	-26.150 -24.714 -23.991	1.00 1.00 1.00	118.22 129.60 129.60
70	7065	CG1	VAL E VAL E	118 118	-21.888 -21.403	72.855 72.044	-23.349 -22.155	1.00 1.00	89.69 60 69

	7066	CG2	VAL E	118	-20.798	72.955	-24.377	1.00	89.69
	7067	C	VAL E	118	-23.869	71.403	-22.939	1.00	129.60
	7068 7069	0	VAL E	118	-24.702	71.913	-22.190	1.00	129.60
5	7070	N CA	ILE E	119	-23.522	70.124	-22.896	1.00	95.90
•	7071	CB	ILE E	119 119	-24.087 -25.146	69.164	-21.965	1.00	95.90
	7072	CG2	ILE E	119	-25.826	68.311 67.375	-22.666	1.00	119.63
	7073	CG1	ILE E	119	-26.147	69.225	-21.651 -23.373	1.00 1.00	119.63
	7074	CD1	ILE E	119	-26.848	68.560	-24.500	1.00	119.63
10	7075	С	ILE E	119	-22.989	68.219	·21.503	1.00	119.63 95.90
	7076	0	ILE E	119	-22.248	67.666	-22.322	1.00	95.90
	7077	N	TYR E	120	-22.869	68.034	-20.202	1.00	107.56
	7078 7079	CA CB	TYR E	120	-21.875	67.106	-19.719	1.00	107.56
15	7080	CG	TYR E TYR E	120	-21.255	67.604	-18.439	1.00	104,01
	7081	CD1	TYR E	120 120	-20.386 -20.926	68.807 70.082	-18.628	1.00	104.01
	7082	CE1	TYR E	120	-20.114	70.062	-18.631 -18.804	1.00	104.01
	7083	CD2	TYR E	120	-19.015	68.678	-18.804	1.00 1.00	104.01
••	7084	CE2	TYR E	120	-18.202	69.795	-18.983	1.00	104.01 104.01
20	7085	CZ	TYR E	120	-18.752	71.061	-18.983	1.00	104.01
	7086	ÓН	TYR E	120	-17.939	72.151	-19.184	1.00	104.01
	7087	C	TYR E	120	-22.604	65.814	-19.436	1.00	107.56
	7088	0	TYR E	120	-23.806	65.843	-19.141		107.56
25	7089 7090	N CA	TYR E	121	-21.908	64.685	-19.536	1.00	107.48
23	7090	CB	TYR E TYR E	121	-22.543	63.401	-19.260	1.00	107.48
	7092	CG	TYR E	121 121	-22.756 -23.773	62.594	-20.561	1.00	135.25
	7093	CD1	TYR E	121	-23.626	63.118 64.371	-21.547	1.00	135.25
	7094	CE1	TYR E	121	-24.513	64.825	-22.119 -23.097	1.00	135.25
30	7095	CD2	TYR E	121	-24.837	62.324	-21.967	1.00 1.00	135.25 135.25
	7096	CE2	TYR E	121	-25.730	62.763	-22.942	1.00	135.25
	7097	CZ	TYR E	121	-25.567	64.011	-23.507	1.00	135.25
	7098	ОН	TYR E	121	-26.438	64.440	-24.498	1.00	135.25
35	7099 7100	C	TYR E	121	-21.708	62.546	-18.293	1.00	107.48
55	7101	N	TYR E LYS E	121 122	-20.476	62.430	-18.440	1.00	107.48
	7102	CA	LYS E	122	-22.376 -21.694	61.938	-17.315	1.00	117.16
	7103	CB	LYS E	122	-21.760	61.059 61.615	-16.384 -14.969	1.00	117.16
	7104	CG	LYS E	122	-21.046	60.734	-13.965	1.00 1.00	184.34 184.34
40	7105	CD	LYS E	122	-21.385	61.133	-12.559	1.00	184.34
	7106	CE	LYS E	122	-20.792	60.167	-11.568	1.00	184.34
	7107	NZ	LYS E	122	-21 .26 6	60.513	-10.209	1.00	184.34
	7108 7109	C	LYS E	122	-22.391	59.709	-16.426	1.00	117.16
45	7110	Ň	LYS E ASP E	122	-23.564	59.597	-16.064	1.00	117.16
	7111	CA	ASP E	123 123	-21.669 -22.228	58.684	-16.864	1.00	145.37
	7112	CB	ASP E	123	-22.532	57.333 56.766	-16.960 -15.574	1.00	145.37
	7113	CG	ASP E	123	-21.271	56.378	-15.574 -14.821	1.00 1.00	150.82
5 0	7114	OD1	ASP E	123	-20.424	55.649	-15.391	1.00	150.82 150.82
50	7115	OD2	ASP E	123	-21.128	56.795	-13.657	1.00	150.82
	7116	C	ASP E	123	-23.483	57.247	-17.825	1.00	145.37
	7117 7118	0	ASP E	123	-24.508	56.696	-17.395	1.00	145.37
	7118	N CA	GLY E	124	-23.389	57.796	-19.040	1.00	162.19
55	7120	c c	GLY E GLY E	124 124	-24.497 -25.683	57.764	-19.983	1.00	162.19
	7121	ŏ	GLY E	124	-26.586	58.666 58.768	-19.698	1.00	162.19
	7122	N	GLU E	125	-25.683	59.324	-20.526 -18.541	1.00	162.19
	7123	CA	GLU E	125	-26.776	60.216	-18.134	1.00 1.00	143.04 143.04
60	7124	CB	GLU E	125	-27.041	60.063	-16.627	1.00	249.69
60	7125	CG	GLU E	125	-27.627	58.724	-16.208	1.00	249.69
	7126	CD	GLU E	125	-29.094	58.592	-16.573	1.00	249.69
	7127 7129	OE1	GLU E	125	-29.901	59.390	-16.051	1.00	249.69
	7128 7129	OE2 C	GLU E GLU E	125	-29.440	57.696	-17.379	1.00	249.69
65	7130	ŏ	GLU E	125 125	-26.510 -25.394	61.692	-18.437	1.00	143.04
	7131	Ň	ALA E	126	-25.384 -27.550	62.166 62.414	-18.309	1.00	143.04
	7132	CA	ALA E	126	-27.350 -27.416	62.414 63.838	-18.843	1.00	144.33
	7133	CB	ALA E	126	-28.693	64.365	-19.120 -19.726	1.00	144.33
70	7134	Ç	ALA E	126	-27.187	64.451	-19.726 -17.754	1.00 1.00	160.82 144.33
70	7135	0	ALA E	126	-27.835	64.054	-16.791	1.00	144.33
							• • •		177.00

	7136	N	LEU E	127	-26.285	65.419	-17.645	1.00	143.63
	7137	CA	LEU E	127	-26.002	65.998	-16.319	1.00	143.63
	7138 7139	CB CG	LEU E	127	-24.565	65.687	-15.904	1.00	101.20
5	7140	CD1	LEU E	127 127	-24.442 -25.446	65.621 64.623	-14.395 -13.859	1.00	101.20
	7141	CD2	LEU E	127	-23.029	65.214	-13.859	1.00 1.00	101.20
	7142	С	LEU E	127	-26.247	JT.484	-16.121	1.00	101.20 143.63
	7143	0	LEU E	127	-27.036	67.875	-15.264	1.00	143.63
10	7144 7145	N CA	LYS E Lys e	128	-25.532	68.305	-16.880	1.00	117.01
10	7146	CB	LYS E LYS E	128 128	-25.707 -24.508	69.747 70.394	-16.812	1.00	117.01
	7147	CG	LYS E	128	-24.263	69.930	-16.141 -14.718	1.00 1.00	217.61
	7148	CD	LYS E	128	-25.300	70.474	-13 748	1.00	217.61 217.61
15	7149	CE	LYS E	128	-24.958	70.073	-12.316	1.00	217.61
15	7150	NZ	LYS E	128	-25.780	70.793	-11 306	1.00	217.61
	7151 7152	C	LYS E LYS E	128	-25.842	70.272	-18.245	1.00	117.01
	7153	Ň	TYR E	128 129	-25.417 -26.424	69.599 71.461	-19.194	1.00	117.01
	7154	CA	TYR E	129	-26.601	2.029	-18.406 -19.736	1.00 1.00	145.51
20	7155	СВ	TYR E	129	-27.928	71.565	-20.322	1.00	145.51 135.80
	7156	CG	TYR E	129	-28.368	72.425	-21.479	1.00	135.80
	7157 7158	CD1 CE1	TYR E	129	-27.913	72.180	-22.768	1.00	135.80
	7159	CD2	TYR E TYR E	129 129	-28.292 -29.214	73.003	-23.829	1.00	135.80
25	7160	CE2	TYR E	129	-29.599	73.521 74.344	-21.273 -22,318	1.00	135.80
	7161	CZ	TYR E	129	-29.135	74.078	-23.595	1.00 1.00	135.80 135.80
	7162	ŌН	TYR E.	129	-29.523	74.878	-24.643	1.00	135.80
	7163	C	TYR E	129	-26.557	73.557	-19.774	1.00	145.51
30	7164 7165	0 N	TYR E TRP E	129	-27.124	74.221	-18.907	1.00	145.51
50	7166	CA	TRP E	130 130	-25.900 -25.786	74.105 75.554	-20.800	1.00	157.70
	7167	CB	TRP E	130	-24.539	76.108	-20.976 -20.279	1.00 1.00	157.70
	7168	CG	TRP E	130	-24.287	75.631	-18.878	1.00	223.39 223.39
35	7169	CD2	TRP E	130	-24.485	76.370	-17.677	1.00	223.39
33	7170 7171	CE2 CE3	TRP E	130	-24.066	75.557	-16.598	1.00	223.39
	7172	CD1	TRP E	130 130	-24.971 -23.782	77.660 74.419	-17.393	1.00	223.39
	7173	NE1	TRP E	130	-23.638	74.364	-18.498 -17.134	1.00 1.00	223.39 223.39
40	7174	CZ2	TRP E	130	-24.117	75.974	-15.268	1.00	223.39
40	7175	CZ3	TRP E	130	-25.023	78.083	-16.063	1.00	223.39
	7176 7177	CH2 C	TRP E	130	-24.605	77.238	-15.018	1.00	223.39
	7178	ŏ	TRP E TRP E	130 130	-25.699 -25.526	75.944 75.103	-22.451	1.00	157.70
	7179	Ň	TYR E	131	-25.812	75.103 77.239	-23.321 -22.718	1.00 1.00	157.70
45	7180	CA	TYR E	131	-25.721	77.775	-24.074	1.00	154.17 154.17
	7181	CB	TYR E	131	-26.551	79.040	-24.193	1.00	200.28
	7182 7183	CG CD1	TYR E	131	-26.730	79.484	-25.605	1.00	200.28
	7184	CE1	TYR E TYR E	131 131	-27.576 -27.722	78.794 79.186	-26.465	1.00	200.28
50	7185	CD2	TYR E	131	-26.028	80.579	-27.789 -26.100	1.00 1.00	200.28 200.28
	7186	CE2	TYR E	131	-26.166	80.979	-27.426	1.00	200.28
	7187	CZ	TYR E	131	-27.012	80.277	-28.267	1.00	200.28
	7188 7189	OH C	TYR E	131	-27.129	80.671	-29.584	1.00	200.28
55	7190	ŏ	TYR E TYR E	131 131	-24.238 -23.462	78.105	-24.250	1.00	154.17
	7191	Ň	GLU E	132	-23.848	77.259 79.340	-24.690 -23.930	1.00 1.00	154.1,
	7192	CA	GLU E	132	-22.436	79.713	-23.979	1.00	210.53 210.53
	7193	CB	GLU E	132	-22.234	81.158	-23.507	1.00	249.69
60	7194 7195	CG CD	GLU E	132	-22.565	82.244	-24.531	1.00	249.69
.	7196	CD OE1	GLU E GLU E	132 132	-21.342	83.062	-24.912	1.00	249.69
	7197	OE2	GLU E	132	-20.307 -21.411	82.939 83.832	-24.219 -25.895	1.00	249.69
	7198	c	GLU E	132	-21.980	78.737	-25.895 -22.905	1.00 1.00	249.69 210.53
<i>_ _ _ _</i>	7199	0	GLU E	132	-22.554	78.723	-21.809	1.00	210.53
65	7200	N	ASN E	133	-20.962	77.929	-23.182	1.00	143.28
	7201 7202	CA CB	ASN E	133	-20.610	76.931	-22.193	1.00	143.28
	7203	CG	ASN E ASN E	133 133	-19.691 -18.215	75.833 76.179	-22.820	1.00	158.57
	7204	OD1	ASN E	133	-17.820	76.179 77.296	-22.850 -23.201	1.00 1.00	158.57
70	7205	ND2	ASN E	133	-17.378	75.183	-22.520	1.00	158.57 158.57
									150.57

	7206	C	ASN E	133	-20.152	77.365	-20.796	1.00	142.20
	7207	0	ASN E	133	-20.202	78.541	-20.431		143.28
	7208	N	HIS E	134	-19.772	76.381	-19.995	1.00	143.28
	7209	CA	HIS E	134	-19.363	76.622		1.00	154.96
5	7210	CB	HIS E	134	-20.574		-18.635	1.00	154.96
•	7211	ČĠ	HIS E			76.432	-17.724	1.00	249.69
		CD2		134	-20.319	76.834	-16.296	1.00	249.69
	7212		HIS E	134	-20.339	76.096	-15.160	1.00	249.69
	7213	ND1	HIS E	134	-19.981	78.107	-15.945	1.00	249.69
10	7214	CE1	HIS E	134	-19.792	78.160	-14.625	1.00	249.69
10	7215	NE2	HIS E	134	-20.003	76.958	-14.134	1.00	
	7216	С	HIS E	134	-18.282	75.617	-18.297	1.00	249.69
	7217	0	HIS E	134	-17.703	74.988	-19.184		154.96
	7218	Ň	ASN E	135				1.00	154.96
	7219	CA	ASN E		-18.018	75.457	-17.009	1.00	128.43
15				135	-17.003	74.531	-16.537	1.00	128.43
15	7220	CB	ASN E	135	-15.677	75 <i>.</i> 279	-16. 366	1.00	226.02
	7221	CG	ASN E	135	-15.086	75.721	-17.696	1.00	226.02
	7222	OD1	ASN E	135	-15.047	74.928	-18.643	1.00	226.02
	7223	ND2	ASN E	135	-14,602	76.963	-17.776	1.00	226.02
	7224	С	ASN E	135	-17,436	73.896	-15.226	1.00	
20	7225	0	ASN E	135	-17.046	74.363	-14.166		128.43
	7226	N	ILE E	136	-18.253	72.842		1.00	128.43
	7227	CA	ILE E	136	-18.788		-15.318	1.00	149.25
	7228	CB	ILE E			72.102	-14.159	1.00	149.25
	7229		ILE E	136	-19.268	70.698	-14.588	1.00	170.48
25		CG2	ILE E	136	-18.140	69.955	-15. 26 6	1.00	170.48
23	7230	CG1	ILE E	136	-19.748	69.897	-13.378	1.00	170.48
	7231	CD1	ILE E	136	-20.169	68.485	-13.726	1.00	170.48
	7232	С	ILE E	136	-17.824	71.949	-12.975	1.00	149.25
	7233	0	ILE E	136	-16.894	71.133	-13.008	1.00	
	7234	N	SER E	137	-18.096	72.718	-11.918		149.25
30	7235	CA	SER E	137	-17.258	72.738		1.00	150.66
-	7236	CB	SER E				-10.724	1.00	150.66
	7237			137	-16.914	74.185	-10.367	1.00	213.03
		og	SER E	137	-16.282	74.247	-9.104	1.00	213.03
	7238	Ç	SER E	137	-17.783	72.047	-9.478	1.00	150.66
25	7239	0	SER E	137	-18.969	72.041	-9.203	1.00	150.66
35	7240	N	ILE E	138	-16.853	71.504	-8.709	1.00	157.82
	7241	CA	ILE E	138	-17.154	70.795	-7.483	1.00	157.82
	7242	CB	ILE E	138	-17.060	69.286	-7.712	1.00	122.12
	7243	CG2	ILE E	138	-17.033	68.548	-6.388		
	7244	CG1	ILE E	138	-18.240	68.834		1.00	122.12
40	7245	CD1	ILE E	138			-8.550	1.00	122.12
	7246	C.	ILE E		-18.110	67.429	-9.027	1.00	122.12
	7247			138	-16.219	71.180	-6.339	1.00	157.82
		0	ILE E	138	-15.000	71.039	-6.435	1.00	157.82
	7248	N	THR E	139	-16.813	71.655	-5.251	1.00	216.52
45	7249	CA	THR E	139	-16.073	72.066	-4.067	1.00	216.52
45	7250	CB	THR E	139	-16.922	73.033	-3.250	1.00	203.55
	7251	OG1	THR E	139	-18.202	72.437	-2.992	1.00	203.55
	7252	CG2	THR E	139	-17.135	74.324	-4.026	1.00	203.55
	7253	С	THR E	139	-15.745	70.839	-3.224	1.00	
	7254	0	THR E	139	-14.637	70.307	-3.273		216.52
50	7255	N	ASN E	140	-16.726	70.402		1.00	216.52
	7256	ČA	ASN E	140			-2.446	1.00	176.56
	7257	CB			-16.589	69.224	-1.603	1.00	176.56
	7258		ASN E	140	-17.543	69. 33 6	-0.405	1.00	249.69
		CG	ASN E	140	-17.486	68.128	0.504	1.00	249.69
55	7259	OD1	ASN E	140	-17.585	66. 992	0.040	1.00	249.69
55	726 0	ND2	ASN E	140	-17.347	68. 36 5	1.805	1.00	249.69
	7261	С	ASI. E	140	-16.974	68.036	-2.490	1.00	176.56
	7262	0	ASN E	140	-18.084	67.989	-3.026	1.00	176.56
	7263	N	ALA E	141	-16.060	67.084	-2.648	1.00	
	7264	CA	ALA E	141	-16.311	65.924			151.69
60	7265	CB	ALA E	141			-3.498	1.00	151.69
••	7266	Č			-15.045	65.594	-4.302	1.00	113.23
			ALA E	141	-16.816	64.665	-2.788	1.00	151.69
	7267	0	ALA E	141	-16.218	64.183	-1.826	1.00	151.69
	7268	N	THR E	142	-17.925	64.133	-3.292	1.00	151.96
	7269	CA	THR E	142	-18.534	62.921	-2.754	1.00	151.96
65	7270	CB	THR E	142	-20.050	62.908	-2.974	1.00	230.06
	7271	OG1	THR E	142	-20.612	64.142	-2.510	1.00	230.06
	7272	CG2	THR E	142	-20.678	61.760	-2.218		
	7273	c _	THR E	142	-17.947			1.00	230.06
	7274	ŏ	THR E	142		61.753	-3.520	1.00	151.96
70	7275	Ň	VAL E	143	-17.415	61.923	-4.625	1.00	151.96
, ,	1213		AWF E	143	-18.040	60.560	-2.949	1.00	131.28

	7276 7277 7278	CA CB CG1	VAL E VAL E VAL E	143 143 143	-17.493 -17.368 -18.738	59.381 58.167 57.589	-3.631 -2.692 -2.393	1.00	131.28 141.04
5	7279 7280 7281	CG2 [*]	VAL E VAL E VAL E	143 143 143	-16.485 -18.402 -17.971	57.127 58.987 58.336	-3.322 -4.781 -5.719	1.00 1.00 1.00 1.00	141.04 141.04 131.28 131.28
10	7282 7283 7284 7285	N CA CB CG	GLU E GLU E GLU E	144 144 144	-19.667 -20.614 -22.048	59.388 59.063 59.323	-4.697 -5.746 -5.298	1.00 1.00 1.00	177.47 177.47 249.69
	7286 7287 7288	CD OE1 OE2	GLU E GLU E GLU E	144 144 144 144	-22.470 -22.694 -23.589 -21.977	58.500 59.353 60.221 59.167	-4.105 -2.886 -2.939 -1.880	1.00 1.00 1.00 1.00	249.69 249.69 249.69
15	7289 7290 7291	C O N	GLU E GLU E ASP E	144 144 145	-20.316 -20.847 -19.467	59.875 59.583 60.895	-6.986 -8.050 -6.851	1.00 1.00 1.00	249.69 177.47 177.47 122.39
20	7292 7293 7294 7295	CA CB CG OD1	ASP E ASP E ASP E ASP E	145 145 145 145	-19.091 -18.410 -19.396 -20.326	61.723 62.997 64.013 64.372	-7.994 -7.532 -7.012 -7.768	1.00 1.00 1.00	122.39 174.03 174.03
	7296 7297 7298	OD2 C O	ASP E ASP E	145 145 145	-19.244 -18.165 -17.996	64.459 60.969 61.363	-5.854 -8.943 -10.098	1.00 1.00 1.00 1.00	174.03 174.03 122.39 122.39
25	7299 7300 7301 7302	N CA CB OG	SER E SER E SER E SER E	146 146 146 146	-17.580 -16.672 -16.037 -15.340	59.870 59.031 57.940	-8.458 -9.263 -8.393	1.00 1.00 1.00	134.53 134.53 131,44
30	7303 7304 7305	C O N	SER E SER E GLY E	146 146 147	-17.412 -18.431 -16.892	58.481 58.362 57.729 58.500	-7.281 -10.418 -10.211 -11.628	1.00 1.00 1.00 1.00	131.44 134.53 134.53 156.93
	7306 7307 7308 7309	CA C O N	GLY E GLY E GLY E THR E	147 147 147	-17.542 -16.839 -15.656	57.888 58.176 58.545	-12.769 -14.083 -14.095	1.00 1.00 1.00	156.93 156.93 156.93
35	7310 7311 7312	CA CB OG1	THR E THR E THR E	148 148 148 148	-17.559 -16.993 -16.985 -18.127	58.006 58.263 56.964 56.934	-15.194 -16.530 -17.380 -18.238	1.00 1.00 1.00 1.00	115.73 115.73 136.83 136.83
40	7313 7314 7315	CG2 C O	THR E THR E THR E	148 148 148	-17.031 -17.755 -18.927	55.746 59.409 59.283	-16.476 -17.266 -17.642	1.00 1.00 1.00	136.83 115.73 115.73
	7316 7317 7318 7319	N CA CB CG	TYR E TYR E TYR E TYR E	149 149 149 149	-17.068 -17.660 -17.292 -17.670	60.533 61.699 62.968 62.986	-17.457 -18.084 -17.301	1.00 1.00 1.00	98.03 98.03 106.49
45	7320 7321 7322 7323	CD1 CE1 CD2 CE2	TYR E TYR E TYR E TYR E	149 149 149	-16.951 -17.293 -18.740	62.244 62.279 63.766	-15.828 -14.885 -13.545 -15.378	1.00 1.00 1.00 1.00	106.49 106.49 106.49 106.49
50	7324 7325 7326	CZ OH C	TYR E TYR E TYR E	149 149 149 149	-19.081 -18.358 -18.715 -17.229	63.812 63.065 63.098 61.914	-14.046 -13.137 -11.815 -19.518	1.00 1.00 1.00 1.00	106.49 106.49 106.49 98.03
55	7327 7328 7329 7330	O N CA CB	TYR E TYR E TYR E TYR E	149 150 150 150	-16.224 -18.002 -17.780 -18.019	61.346 62.767 63.194 62.028	-19.972 -20.200 -21.595	1.00 1.00 1.00	98.03 87.55 87.55
	7331 7332 7333	CG CD1 CE1	TYR E TYR E TYR E	150 150 150	-19.456 -20.224 -21.551	61.684 62.527 62.200	-22.591 -22.936 -23.739 -24.087	1.00 1.00 1.00 1.00	125.81 125.81 125.81 125.81
60	7334 7335 7336 .7337	CD2 CE2 CZ OH	TYR E TYR E TYR E TYR E	150 150 150 150	-20.041 -21.371 -22.116 -23.405	60.496 60.157 61.018 60.699	-22.482 -22.828 -23.631	1.00 1.00 1.00	125.81 125.81 125.81
65	7338 7339 7340	C O N	TYR E TYR E CYS E	150 150 151	-18.765 -19.801 -18.456	64.338 64.418 65.235	-23.991 -21.835 -21.160 -22.763	1.00 1.00 1.00 1.00	125.81 87.55 87.55 108.53
	7341 7342 7343 7344	CA C O CB	CYS E CYS E CYS E	151 151 151 151	-19.370 -19.724 -19.030 -18.749	66.343 66.457 65.919	-23.043 -24.522 -25.385	1.00 1.00 1.00	108.53 108.53 108.53
70	7345	SG	CYS E	151	-17.166	67.647 68.090	-22.588 -23.414	1.00 1.00	127.42 127.42

	7346	N	THR E	100	00.040	07.454			
	7347	CA	THR E	152	-20.816	67.151	-24.810	1.00	109.73
	7348	CB:	THR E	152 152	-21.249	67.343	-26.184	1.00	109,73
•	7349	OG1	THR E	152	-22.546 -23.649	66.577	-26.478	1.00	160.87
5	7350	CG2	THR E	152	-23.648 -22.443	67.242 65.158	-25.840	1.00	160.87
	7351	C	THR E	152	-21.530	68.832	-25.963	1.00	160.87
	7352	ŏ	THR E	152	-21.983	69.541	-26.420 -25.509	1.00	109.73
	7353	Ň	GLY E	153	-21.284	69.305	-23.509	1.00	109.73
	7354	CA	GLY E	153	-21.530	70.706	-27.927	1.00	146.21
10	7355	C	GLY E	153	-21.486	71.046	-29.398	1.00 1.00	146.21
	7356	Ō	GLY E	153	-21.040	70.244	-30.204	1.00	146.21
	7357	N	LYS E	154	-21.947	72.247	-29.739	1.00	146.21
	7358	CA	LYS E	154	-21.973	72.704	-31.114	1.00	118.16
	7359	CB	LYS E	154	-23.332	73.316	-31.423	1.00	118.16 235.84
15	7360	CG	LYS E	154	-23.517	73.732	-32.861	1.00	235.84
	7361	CD	LYS E	154	-24.925	74.260	-33.087	1.00	235.84
	7362	CE	LYS E	154	-25.120	74.744	-34.517	1.00	235.84
	7363	NZ	LYS E	154	-26.493	75.280	-34.746	1.00	235.84
	7364	С	LYS E	154	-20.864	73.716	-31.376	1.00	118.16
20	7365	0	LYS E	154	-20.821	74.780	-30.758	1.00	118.16
	7366	N	VAL E	155	-19.957	73.364	-32.288	1.00	164.34
	7367	CA	VAL E	155	-18.825	74.214	-32.686	1.00	164.34
	7368	CB	VAL E	155	-17.520	73.384	-32.768	1.00	138.01
25	7369	CG1	VAL E	155	-16.369	74.233	-33.254	1.00	138.01
25	7370	CG2	VAL E	155	-17.198	72.808	-31.398	1.00	138.01
	7371	Ç	VAL E	155	-19.166	74.746	-34.073	1.00	164.34
	7372	0	VAL E	155	-19.503	73.962	-34.965	1.00	164.34
	7373	N.	TRP E	156	-19.058	76.060	-34.268	1.00	249.37
20	7374	CA	TRP E	156	-19.413	76.665	-35.557	1.00	249.37
30	7375	CB	TRP E	156	-18.639	76.057	-36.746	1.00	249.69
	7376	CG	TRP E	156	-17.160	76.335	-36.808	1.00	249.69
	7377	CD2	TRP E	156	-16.521	77.599	· -37.045	1.00	249.69
	7378 7379	CE2 CE3	TRP E	156	-15.126	77.369	-37.030	1.00	249.69
35	7380	CD1	TRP E	156	-16.992	78.898	-37.283	1.00	249.69
33	7381	NE1	TRP E	156	-16.152	75.425	-36.653	1.00	249.69
	7382	CZ2	TRP E	156	-14.929	76.035	-36.786	1.00	249.69
	7383	CZ3	TRP E	156 156	-14.197	78.389	-37.233	1.00	249.69
	7384	CH2	TRP E	156	-16.067	79.915	-37.486	1.00	249.69
40	7385	C	TRP E	156	-14.684 -20.881	79.652 76.332	-37.459	1.00	249.69
	7386	ŏ	TRP E	156	-21.762	77.001	-35.750	1.00	249.37
	7387	Ň	GLN E	157	-21.128	75.279	-35.194 -36.536	1.00	249.37
	7388	CA	GLN E	157	-22.489	74.837	-36.802	1.00 1.00	132.72
	7389	CB	GLN E	157	-23.006	75.460	-38.103	1.00	132.72
45	7390	CG	GLN E	157	-23.387	76.941	-37.974	1.00	249.69 249.69
	7391	CD	GLN E	157	-24.572	77.181	-37.037	1.00	249.69
	7392	OE1	GLN E	157	-25.685	76.713	-37.291	1.00	249.69
	7393	NE2	GLN E	157	-24.334	77.914	-35.949	1.00	249.69
50	7394	С	GLN E	157	-22.668	73.317	-36.834	1.00	132.72
50	7395	0	GLN E	157	-23.628	72.812	-37.423	1.00	132.72
	7396	Ņ	LEU E	158	-21.756	72.587	-36.195	1.00	229.55
	7397	CA	LEV E	158	-21.863	71.130	-36.137	1.00	229.55
	7398	CB	LEU E	158	-20.818	70.467	-37.038	1.00	228.12
55	7399	CG	LEU E	158	-21.063	70.461	-38.553	1.00	228.12
55	7400	CD1	LEU E	158	-20.552	69.140	-39.108	1.00	228.12
	7401	CD2	LEU E	158	-22.544	70.590	-38.874	1.00	238.12
	7402	Ç	LEU E	158	-21.716	70.605	-34.713	1.00	229.55
	7403	0	LEU E	158	-21.041	71 <i>.</i> 216	-33.88 5	1.00	229.55
60	7404	N	ASP E	159	-22.357	69.472	-34.438	1.00	199.14
00	7405	CA	ASP E	159	-22.299	68.862	-33.114	1.00	199.14
	7406	CB	ASP E	159	-23.567	68.050	-32.848	1.00	198.75
	7407	CG CC1	ASP E	159	-24.829	68.854	-33.075	1.00	198.75
	7408 7409	OD1	ASP E	159	-25.033	69.866	-32.365	1.00	198.75
65	7409 7410	OD2	ASP E	159	-25.613	68.475	-33.970	1.00	198.75
05	7411	CO	ASP E	159	-21.082	67.948	-32.988	1.00	199.14
	7412	N	ASP E	159	-20.656	67.333	-33.963	1.00	199.14
	7413	CA	TYR E TYR E	160	-20.522	67.867	-31.784	1.00	164.98
	7414	CB	TYR E	160 160	-19.368 -19.071	67.017	-31.543	1.00	164.98
70	7415	ČG	TYR E	160	-18.071 -17.950	67.782 69.445	-31.730	1.00	170.02
. •			IIN E	100	-17.959	68.445	-33.079	1.00	170.02

	7416	CD1	TVD E	100	40.400	22.742			
	7417	CE1	TYR É TYR E	160 160	-18.428 -18.291	69.746 70.376	-33.285	1.00	170.02
	7418	CD2	TYR E	160	-17.362	67.787	-34.516 -34.147	1.00 1.00	170.02
_	7419	CE2	TYR E	160	-17.221	68.407	-35.390	1.00	170.02 170.02
5	7420	CZ	TYR E	160	-17.685	69.700	-35.562	1.00	170.02
	7421	ÓН	TYR E	160	-17.517	70.325	-36.771	1.00	170.02
	7422	C	TYR E	160	-19.385	66.416	-30.153	1.00	164.98
	7423 7424	N	TYR E GLU E	160	-19.844	67.025	-29.185	1.00	164.98
10	7425	CA	GLU E	161 161	-18.861 -18.805	65.204 64.435	-30.073	1.00	121.76
	7426	CB	GLU E	161	-19.432	63.056	-28.835 -29.104	1.00 1.00	121.76
	7427	CG	GLU E	161	-19.437	62.062	-27.962	1.00	238.30 238.30
	7428	CD	GLU E	161	-20.385	60.898	-28.227	1.00	238.30
15	7429	OE1	GLU E	161	-20.217	59.834	-27.596	1.00	238.30
15	7430 7431	OE2	GLU E	161	-21.310	61.051	-29.058	1.00	238.30
	7431	C	GLU E	161 161	-17.340	64.330	-28.425	1.00	121.76
	7433	Ň	SER E	162	-16.464 -17.079	64.228 64.384	-29.275 -27.125	1.00	121.76
	7434	CA	SER E	162	-15.712	64.316	-26.603	1.00 1.00	141.30 141.30
20	7435	CB	SER E	162	-15.579	65.188	-25.350	1.00	137.77
	7436	og.	SER E	162	-16.423	64.719	-24.305	1.00	137.77
	7437	C	SER E	162	-15.318	62.905	-26.240	1.00	141.30
	7438 7439	O N	SER E GLU E	162	-16.181	62.046	-26.067	1.00	141.30
25	7440	CA	GLU E	163 163	-14.015 -13.553	62.662 61.335	-26.132	1.00	137.45
	7441	CB	GLU E	163	-12.021	61.264	-25.739 -25.770	1.00 1.00	137.45
	7442	CG	GLU E	163	-11.400	61.173	-27.169	1.00	249.69 249.69
	7443	CD	GLU E	163	-11.585	59.804	-27.826	1.00	249.69
20	7444	OE1	GLU E	163	-11.171	58.791	-27.226	1.00	249.69
30	7445	OE2	GLU E	163	-12.138	59.742	-28.944	1.00	249.69
	7446 7447	C O	GLU E	163 163	-14.057	61.170	-24.309	1.00	137.45
	7448	N	PRO E	164	-14.182 -14.377	62.171 59.935	-23.593	1.00	137.45
	7449	CD	PRO E	164	-14.382	58.681	-23.877 -24.662	1.00 1.00	95.03 218.77
35	7450	CA	PRO E	164	-14.877	59.684	-22.521	1.00	95.03
	7451	CB	PRO E	164	-15.570	58.345	-22.657	1.00	218.77
	7452	ÇG	PRO E	164	-14.657	57.637	-23.594	1.00	218.77
	7453 7454	C O	PRO E PRO E	164 164	-13.761	59.664	-21.475	1.00	95.03
40	7455	Ň	LEU E	165	-12.660 -14.046	59.202 60.133	-21.764	1.00	95.03
	7456	CA	LEU E	165	-13.021	60.175	-20.267 -19.240	1.00 1.00	132.61 132.61
	7457	CB	LEU E	165	-12.581	61.627	-19.014	1.00	87.30
	7458	CG	LEU E	165	-11.475	61.851	-17.979	1.00	87.30
45	7459	CD1	LEU E	165	-10.446	60.707	-18.043	1.00	87.30
43	7460 7461	CD2 C	LEU E LEU E	165	-10.812	63.181	-18.220	1.00	87.30
	7462	ŏ	LEU E	165 165	-13.411 -14.470	59.560 59.883	-17.905	1.00	132.61
	7463	Ň	ASN E	166	-12.545	58.690	-17.367 -17.364	1.00 1.00	132.61 112.66
	7464	CA	ASN E	160	-12.794	58.050	-16.068	1.00	112.66
50	7465	CB	ASN E	166	-12.116	56.693	-16.002	1.00	172.55
	7466	CG	ASN E	166	-13.038	55.560	-16.402	1.00	172.55
	7467 7469	OD1	ASN E	166	-14.264	55.679	-16.328	1.00	172.55
	7468 7469	ND2 C	ASN E	166 166	-12.445 -12.294	54.443	-16.804	1.00	172.55
55	7470	ŏ	ASN E	166	-11.246	58.889 ა9.511	-14.909 -14.999	1.00	112.66
	7471	N	II.E E	167	-13.032	58.887	-13.807	1.00 1.00	112.66 147.51
	7472	CA	ILE E	167	-12.643	59.658	-12.628	1.00	147.51
	7473	CB	ILE E	167	-13.409	60.966	-12.546	1.00	109.60
60	7474 7475	CG2	ILE E	167	-13.051	61.688	-11.260	1.00	109.60
00	7475 7476	CG1 CD1	ILE E	167 167	-13.086	61.820	-13.760	1.00	109.60
	7477	Č	ILE E	167	-13.847 -12.904	63.089 58.901	-13.806 -11.343	1.00	109.60
	7478	Ŏ	ILE E	167	-14.007	58.401	-11.345	1.00 1.00	147.51 147.51
	7479	N	THR E	168	-11.903	58.840	-10.481	1.00	104.75
65	7480	CA	THR E	168	-12.093	58.106	-9.251	1.00	104.75
	7481	CB	THR E	168	-11.250	56.819	-9.263	1.00	148.63
	7482 7483	OG1 CG2	THR E	168	-11.607	56.040	-10.408	1.00	148.63
	7484	C	THR E	168 168	-11.516	55.997 50.000	-8.014 7.050	1.00	148.63
70	7485	ŏ	THR E	168	-11.831 -10.763	58.886 59.432	-7.956 -7.718	1.00 1.00	104.75
							7.710	1.00	104.75

	7400	A1							
	7486 7487	N	VAL E	169	-12.849	58.924	-7.117	1.00	128.03
	7487 7488	CA CB	VAL E	169	-12.771	59.592	-5.835	1.00	128.03
	7489	CG1	VAL E	169	-14.028	60.478	-5.592	1.00	104.73
5	7490	CG2	VAL E	169 169	-14.231	60.741	-4.125	1.00	104.73
	7491	C	VAL E	169	-13.853 -12.683	61.798 58.492	-6.296	1.00	104.73
	7492	ŏ	VAL E	169	-12.665	57.767	-4.783 4.542	1.00	128.03
	7493	Ň	ILE E	170	-11.510	58.363	-4.542	1.00	128.03
	7494	CA	ILE E	170	-11.265	57.356	-4.171 -3.135	1.00	164.43
10	7495	CB	ILE E	170	-9.826	56.804	-3.135	1.00	164.43
	7496	CG2	ILE E	170	-9.566	56.357	-4.685	1.00 1.00	148.98
	7497	CG1	ILE E	170	-8.816	57.897	-2.906	1.00	148.98
	7498	CD1	ILE E	170	-7.368	57. 44 0	-2.961	1.00	148.98
	7499	С	ILE E	170	-11.467	57.968	-1.744	1.00	148.98 164.43
15	7500	0	ILE E	170	-11.524	59.184	-1.610	1.00	164.43
	7501	N	LYS E	171	-11.560	57.141	-0.709	1.00	181.58
	7502	CA	LYS E	171	-11.775	57.672	0.633	1.00	181.58
	7503	CB	LYS E	171	-13.118	57.176	1.157	1.00	249.69
	7504	CG	LYS E	171	-13.230	55.666	1.123	1.00	249.69
20	7505	CD	LYS E	171	-14.675	55.211	0.996	1.00	249.69
	75 06	CE	LYS E	171	-15.530	55.712	2.154	1.00	249.69
	75 07	NZ	LYS E	171	-16.931	55.206	2.058	1.00	249.69
	7508	Ç	LYS E	171	-10.673	57.327	1.632	1.00	181.58
25	7509	0	LYS E	171	·-10.810	57.585	2.833	1.00.	181.58
25	7510	C1	NAG E	221	2.209	79.546	-26.386	1.00	249.69
	7511	C2	NAG E	221	0.889	80.273	-26.643	1.00	249.69
	7512	N2	NAG E	221	-0.170	79.298	-26.828	1.00	249.69
	7513	C7	NAG E	221	-1.431	79.634	-26.596	1.00	249.69
30	7514	07	NAG E	221	-1.768	80.762	-26.235	1.00	249.69
30	7515	C8 ·	NAG E	221	-2.476	78.553	-26.806	1.00	249.69
	7516	C3	NAG E	221	1.001	81.165	-27.881	1.00	249.69
	7517 7510	O3	NAG E	221	-0.178	81.953	-28.009	1.00	249.69
	7518 7519	C4 O4	NAG E	221	2.237	82.087	-27.816	1.00	249.69
35	7520	C5	NAG E NAG E	221	2.396	82.690	-29.116	1.00	249.69
55	7521	O5	NAG E	221	3.502	81.275	-27.447	1.00	249.69
	7522	C6	NAG E	221 221	3.276 4.726	80.502	-26.244	1.00	249.69
	7523	06	NAG E	221	4.477	82.136 83.098	-27.185	1.00	249.69
	7524	C1	NAG E	222	3.181	83.831	-26.171 -29.256	1.00	249.69
40	7525	C2	NAG E	222	2.456	84.839	-30.180	1.00 1.00	249.69
	7526	N2	NAG E	222	1.186	85.239	-29.587	1.00	249.69
	7527	C7	NAG E	222	0.936	86.518	-29.301	1.00	249.69 249.69
	7528	07	NAG E	222	1.741	87.429	-29.516	1.00	249.69 249.69
	7529	C8	NAG E	222	-0.420	86.835	-28.681	1.00	249.69
45	7530	C3	NAG E	222	2.220	84.191	-31.568	1.00	249.69
	7531	O 3	NAG E	222	1.662	85.147	-32.469	1.00	249.69
	7532	C4	NAG E	222	3.543	83.638	-32.143	1.00	249.69
	7533	O4	NAG E	222	3.281	82.909	-33.338	1.00	243.69
50	7534	C5	NAG E	22 2	4.233	82.718	-31.115	1.00	249.69
50	7535	Q 5	NAG E	222	4.427	83.426	-29.859	1.00	249.69
	7536	C6	NAG E	222	5.592	82.211	-31.572	1.00	249.69
	7537	06	NAG E	22 2	5.701	80.806	-31.409	1.00	249.69
	7538	C1	NAG E	242	7.147	59.017	-23.850	1.00	193.96
55	7539	C2	NAG E	242	7.463	59.646	-25.212	1.00	193.96
<i>J J</i>	7540	N2	NAG E	242	8.286	60.830	-25.064	1.00	193.96
	7541 7542	C7	NAG E	242	9.478	60.868	-25.645	1.00	1ຍປ.96
	7542 7543	O7 C8	NAG E	242	9.927	59.930	-26.305	1.00	193.96
	7544	င္ဖ	NAG E	242	10.299	62.130	-25.465	1.00	193.96
60	7545	03	NAG E NAG E	242	6.151	59.995	-25.913	1.00	193.96
00	7546	C4	NAG E	242 242	6.418	60.545	-27.194	1.00	193.96
	7547	04	NAG E	242	5.284	58.740	-26.060	1.00	193.96
	7548	C5	NAG E	242 242	3.983 5.124	59.116	-26.566	1.00	193.96
	7549	O5	NAG E	242 242	5.124 6.411	58.005 57.700	-24.698 -24.050	1.00	193.96
65	7550	C6	NAG E	242	4.509	57.799 56.624	-24.050 -24.872	1.00	193.96
	7551	06	NAG E	242	3.211	56.550		1.00	193.96
	7552	C1	NAG E	243	3.598	58.568	-24.304 -27.770	1.00	193.96
	7553	C2	NAG E	243	2.085	58.638	-27.770 -27.907	1.00	215.12
	7554	N2	NAG E	243	1.433	57.909	-27.807 -26.843	1.00	215.12
70	7555	C7	NAG E	243	0.428	58.482	-26.182	1.00 1.00	215.12 215.12
			·- -				-0.102	1.00	Z13.12

	7556	07	NAG E	243	0.027	59.633	-26.423	1.00	215.12
	7557	C8	NAG E	243	-0.230	57.665	-25.075	1.00	215.12
	7558	C3 .	NAG E	243	1.685	58.056	-29.247	1.00	215.12
_	7559	03	NAG E	243	0.272	58.105	-29.401	1.00	
5	7560	C4	NAG E	243	2.344	58.866	-30.339	1.00	215.12
	7561	04	NAG E	243	1.898	58.318	-31.574	1.00	215.12
	7562	C5	NAG E	243	3.883	58.823	-30.140	1.00	215.12
	7563	O 5	NAG E	243	4.208	59.328	-28.814	1.00	215.12
	7564	C6	NAG E	243	4.624	59.699	-31.116	1.00	215.12
10	7565	06	NAG E	243	4.268	61.057	-30.933		215.12
	7566	C1	MAN E	244	1.748	59.080	-32.701	1.00	215.12
	7567	C2	MAN E	244	2.233	58.170	-32.701	1.00	219.74
	7568	02	MAN E	244	1.708	56.848	-33.490	1.00	219.74
	7569	C3	MAN E	244	1.963	58.748	-35.107	1.00	219.74
15	7570	03	MAN E	244	2.548	57.949	-36.119	1.00	219.74
	7571	C4	MAN E	244	0.488	58.983	-35.314	1.00	219.74
	7572	04	MAN E	244	0.264	59.475		1.00	219.74
	7573	C5	MAN E	244	0.038	59.992	-36.620 -34.253	1.00	219.74
	7574	O5	MAN E	244	0.282	59.4		1.00	219.74
20	7575	C6	MAN E	244	-1.419	60.489	-32.908	1.00	219.74
	7576	06	MAN E	244	-2.389		-34.434	1.00	219.74
	7577	C1	NAG E	250	12.894	59.610 70.616	-33.877	1.00	219.74
	7578	C2	NAG E	250 250		79.616	-14.981	1.00	249.69
	7579	N2			12.331	80.923	-14.392	1.00	249.69
25	7580	C7	NAG E	250	12.256	80.832	-12.946	1.00	249.69
23	7581	07	NAG E	250	13.100	81.532	-12.196	1.00	249.69
	7582	C8	NAG E	250	13.967	82.276	-12.673	1.00	249.69
	7583	ငဒ	NAG E	250	12.966	81.387	-10.683	1.00	249.69
	7584		NAG E	250	10.934	81.188	-14.970	1.00	249.69
30	7585	03	NAG E	250	10.442	82.440	-14.506	1.00	249.69
50	7586	C4	NAG E	250	10.987	81.183	-16.508	1.00	249.69
	7587	O4	NAG E	250	9.667	81.305	-17.032	1.00	249.69
	7588	C5	NAG E	250	11.643	79.872	-17.010	1.00	249.69
	7589	O5	NAG E	250	12.954	79.705	-16.412	1.00	249.69
35	7590	C6	NAG E	250	11.833	79.816	-18.522	1.00	249.69
33	7590 7591	O6	NAG E	250	12.752	78.791	-18.892	1.00	249.69
	7592	C1	NAG E	274	14.635	58.650	0.211	1.00	249.69
		C2	NAG E	274	13.525	58.145	1.158	1.00	249.69
	7593	N2	NAG E	274	13.058	59.230	2.009	1.00	249.69
40	7594 7595	C7	NAG E	274	11.826	59.208	2.513	1.00	249.69
70	7596	O7	NAG E	274	11.030	58.289	2.302	1.00	249.69
		C8	NAG E	274	11.415	60.380	3.387	1.00	249.69
	7597 7500	ය	NAG E	274	14.058	56.984	2.020	1.00	249.69
	7598	03	NAG E	274	12.997	56.422	2.785	1.00	249.69
45	7599	C4	NAG E	274	14.687	55.894	1.134	1.00	249.69
43	7600	O4	NAG E	274	15.298	54.900	1.951	1.00	249.69
	7601	C5	NAG E	274	15.736	56.513	0.196	1.00	249.69
	7602	O5	NAG E	274	15.136	57.567	-0.595	1.00	249.69
	7603	C6	NAG E	274	16.324	55.500	-0.775	1.00	249.69
50	7604	O6	NAG E	274	17.151	56.129	-1.748	1.00	249.69
20	7605	C1	NAG E	335	-13.218	77.155	-18.184	1.00	248.99
	7606	C2	NAG E	335	-12.377	77.952	-17.147	1.00	248.99
	7607	N2	NAG E	335	-13.025	77.859	-15.850	1.00	248.99
	7608	C7	NAG E	335	-12.415	77.253	-14.835	1.00	248.99
55	7609	07	NAG E	335	-11.291	76.751	-14.921	1.00	248.99
55	7610	C8	NAG E	335	-13.169	77.199	-13.517	1.00	248.99
	7611	C3	NAG E	335	-12.169	79.444	-17.498	1.00	248.99
	7612	O3 .	NAG E	335	-11.051	79.949	-16.774	1.00	248.99
	7613	C4	NAG E	335	-11.918	79.636	-18.990	1.00	248.99
60	7614	04	NAG E	335	-11.812	81.021	-19.294	1.00	248.99
60	7615	C5	NAG E	335	-13.079	79.014	-19.748	1.00	248.99
	7616	O5	NAG E	335	-13.060	77.584	-19.562	1.00	248.99
	7617	C6	NAG E	335	-12.991	79.270	-21.238	1.00	248.99
	7618	O6	NAG E	335	-14.176	79.882	-21.722	1.00	248.99
<i>C</i> =	7619	C1	NAG E	340	-18.408	67.970	2.712	1.00	249.69
65	7620	C2	NAG E	340	-17.972	66.798	3.606	1.00	249.69
	7621	N2	NAG E	340	-17.526	65.688	2.783	1.00	249.69
	7622	C7	NAG E	340	-16.380	65.065	3.055	1.00	249.69
	7623	07	NAG E	340	-15.644	65.372	4.003	1.00	249.69
	7624	C8	NAG E	340	-15.987	63.917	2.140	1.00	249.69
70	7625	C3	NAG E	340	-19.162	66.374	4.487	1.00	249.69
				-				1.00	245.03

	7626	03	NAG E	340	-18.769	65.355	5.395	1.00	249.69
	7627	C4	NAG E	340	-19.704	67.580	5.273	1.00	249.69
	7628	O4 [*]	NAG E	340	-20.884	67.199	5.975	1.00	249.69
_	7629	C5	NAG E	340	-20.011	68.748	4.305	1.00	249.69
5	7630	O 5	NAG E	340	-18.836	69.073	3.520	1.00	249.69
	7631	C6	NAG E	340	-20.450	70.028	5.000	1.00	249.69
	7632	O6	NAG E	340	-20.520	71.112	4.081	1.00	249.69
	7633	C1	NAG E	366	-13.236	53.354	-17.338	1.00	200.99
	7634	C2	NAG E	366	-12.501	52.697	-18.503	1.00	200.99
10	7635	N2	NAG E	366	-12.267	53.689	-19.539	1.00	200.99
	7636	C7	NAG E	366	-11,142	54.405	-19.544	1.00	200.99
	7637	07	NAG E	366	-10.251	54.258	-18.697	1.00	200.99
	7638	C8	NAG E	366	-10.974	55.435	-20.659	1.00	200.99
	7639	сз	NAG E	366	-13.344	51.559	-19.064	1.00	200.99
15	7640	O3	NAG E	366	-12.589	50.845	-20.024	1.00	200.99
	7641	C4	NAG E	366	-13.814	50.601	-17.968	1.00	200.99
	7642	04	NAG E	366	-14.809	49.714	-18.523	1.00	200.99
	7643	C5	NAG E	366	-14.427	51.387	-16.796	1.00	200.99
	7644	O5	NAG E	366	-13.511	52.389	-16.333	1.00	200.99
20	7645	C6	NAG E	366	-14.780	50.532	-15.594	1.00	200.99
	7646	O6	NAG E	366	-15.500	51.287	-14.628	1.00	200.99
	7647	C1	NAG E	367	-14.595	48.351	-18.366	1.00	248.88
	7648	C2	NAG E	367	-15.915	47.598	-18.528	1.00	248.88
	7649	N2	NAG E	367	-16.897	48.084	-17.575	1.00	248.88
25	7650	C7	NAG E	367	-17.964	48.748	-18.004	1.00	248.88
	7651	07	NAG E	367	-18.175	48.977	-19.195	1.00	248.88
	7652	C8	NAG E	367	-18.948	49.229	-16.950	1.00	248.88
	7653	C3	NAG E	367	-15.646	46.102	-18.325	1.00	248.88
	7654	03	NAG E	367	-16.851	45.362	-18.485	1.00	248.88
30	7655	C4	NAG E	367	-14.602	45.631	-19.346	1.00	248.88 248.88
-	7656	04	NAG E	367	-14.273	44.271	-19.099	1.00	248.88
	7657	C5	NAG E	367	-13.334	46.502	-19.256	1.00	248.88 248.88
	7658	O5	NAG E	367	-13.668	47.911	-19.373	1.00	248.88 248.88
	7659	C6	NAG E	367	-12.347	46.188	-20.363	1.00	248.88
35	7660	06	NAG E	367	-12.226	47.271	-21.276	1.00	248.88
						71.61	-21.210	1.00	£40.00

Table 7. Atomic coordinates of PhFceRI α_{1-176} , Form M2

	ATOM NUMBER	ATOM TYPE	RESIDUE		_X_	<u>_Y_</u>	_Z_	<u>000</u>	B
	1	СВ	VAL A	1	54.132	-20.714	0.400		
5	2	CG1	VAL A	i	52.843	-21.062	8.499 7.774	1.00 1.00	178.10
	3	CG2	VAL A	1	54.598	-21.899	9.342	1.00	175.86 170.07
	4	C	VAL A	1	55.044	-18.854	6.922	1.00	182.13
	5 6	0 N	VAL A	1	54.219	-18.626	6.045	1.00	181.45
10	7	CA	VAL A VAL A	1	56.560 55.237	-20.445 -20.291	8.067	1.00	185.40
	8	N	PRO A	2	55.807	-17.881	7.470 7.435	1.00 1.00	181.27
	9	CD	PRO A	2	55.929	-17.840	8.889	1.00	180.05 177.25
	10	CA	PRO A	2	55.680	-16.493	6.950	1.00	173.64
15	11 12	CB CG	PRO A	2	56.618	-15.752	7.867	1.00	173.09
13	13	C	PRO A PRO A	2	56.407 55.836	-16.439 -16.175	9.184	1.00	173.72
	14	ŏ	PRO A	2	55. 605	-15.044	5.460 5.015	1.00 1.00	167.05
	15	N	GLN A	3	56.252	-17.165	4.696	1.00	168.35 154.29
20	16	CA	GLN A	3	56.695	-17.039	3.302	1.00	144.07
20	17 18 .	CB CG	GLN A	3	56.716	-18.462	2.775	1.00	152.72
	19	CD	GLN A GLN A	3 3	57.593 58.812	-19.352	3.656	1.00	159.56
	20	OE1	GLN A	3	58.812 59.151	-18.642 -17.549	4.253	1.00	162.34
	21	NE2	GLN A	3	59.600	-19.090	3.808 5.219	1.00 1.00	167.23
25	22	С	GLN A	3	56.117	-15.992	2.286	1.00	166.20 134.57
	23	0	GLN A	3	56.663	-15.988	1.196	1.00	145.79
	24	N	LYS A	4	55.146	-15.111	2.520	1.00	114.68
	25 26	CA CB	LYS A Lys a	4	54.768	-14.237	1.357	1.00	91.89
30	27	CG	LYS A	4	53.529 52.415	-14.805 -15.272	0.655 1.595	1.00	93.44
	28	CD	LYS A	4	51.061	-15.271	0.914	1.00 1.00	116.31 123.93
	29	CE	LYS A	4	50.072	-16.156	1.643	1.00	131.64
	30	NZ	LYS A	4	49.049	-16.742	0.732	1.00	135.93
35	31 32	C O	LYS A	4	54.546	-12.760	1.718	1.00	72.33
55	33	N	LYS A PRO A	4	54.002 54.961	-12.486 -11.818	2.790	1.00	69.94
	34	CD	PRO A	5 5	55.670	-12.005	0.861 -0.413	1.00 1.00	46.80
	35	CA	PRO A	5	54.807	-10.400	1.180	1.00	34.03 35.08
40	36	CB	PRO A	5	55.351	-9.708	-0.066	1.00	27.27
40	37 38	CG	PRO A	5	56.350	-10.674	-0.591	1.00	18.92
	39	С О	PRO A PRO A	5 5	53.320	-10.124	1.371	1.00	41.36
	40	N	LYS A	6	52.473 52.988	-10.945 -8.970	1. 030 1.915	1.00	59.20
	41	CA	LYS A	6	51.591	-8.644	2.112	1.00 1.00	45.12 58.01
45	42	CB	LYS A	6	51.207	-8.907	3.570	1.00	31.24
	43	CG	LYS A	6	49.726	-8.775	3.844	1.00	63.36
	44 45	CD CE	LYS A	6	49.203	-10.005	4.566	1.00	81.81
	46 46	NZ	LYS A LYS A	6 6	47.699 47.156	-9.917	4.797	1.00	83.24
50	47	C	LYS A	6	51.392	-11.172 -7.177	5.406 1.734	1.00 1.00	80.30
	48	Ō	LYS A	6	51.822	-6.280	2.460	1.00	61.99 80.08
	49	N	VAI A	7	50.773	-6.936	0.583	1.00	46.06
	50	CA	VAL A	7	50.542	-5 <i>.</i> 574	0.153	1.00	39.39
55	51 52	CB CG1	VAL A VAL A	7	49.937	-5.529	-1.254	1.00	45.45
55	53	CG2	VAL A	7 7	49.551 50.947	-4.097 -6.057	-1.603	1.00	49.77
	54	C	VAL A	7	49.594	-4.890	-2.270 1.125	1.00 1.00	22.27 44.09
	55	0	VAL A	7	48.558	-5.446	1.493	1.00	37.53
60	56	N	SER A	8	49.970	-3.686	1.546	1.00	52.74
60	57 58	CA	SER A	8	49.162	-2.909	2.474	1.00	53,44
	59	CB OG	SER A SER A	8	49.936	-2.627	3.752	1.00	61.38
	60	C	SER A	8 8	50. 799 48.886	-1.517 -1.598	3.558 1.772	1.00	88.92
	61	0	SER A	8	49.698	-1.134	0.963	1.00 1.00	51.41 45.35
65	62	N	LEU A	9	47.753	-0.988	2.080	1.00	44.36
	63	CA	LEU A	9	47.422	0.260	1.422	1.00	49.82
	64	СВ	LEU A	9	46.027	0.193	0.778	1.00	64.30

	65 66	CG CD1	LEU A	9 .	45.511 44.236	-1.067 -0.713	0.680	1.00	48.97
	67	CD2	LEU A	9	46.536	-1.600	-0.646	1.00	42.71
_	68	C	LEU A	9	47.429	1.408	-0.898 2.405	1.00 1.00	20.50
5	69	0	LEU A	9	47.003	1.263	3.551	1.00	39.97
	70	N	ASN A	10	47.892	2.557	1.937	1.00	31.04 39.17
	71	CA	ASN A	10	47.888	3.747	2.758	1.00	38.83
	72 73	CB	ASN A	10	49.249	3.992	3.387	1.00	56.48
10	73 74	CG OD1	ASN A	10	49.281	5.278	4.188	1.00	70.12
10	7 5	ND2	ASN A ASN A	10 10	48.500	5.445	5.135	1.00	58.68
	76	C	ASN A	10	50.169 47.518	6.205 4.957	3.807	1.00	68.79
	77	Ö	ASN A	10	48.302	5.400	1.909 1.040	1.00	31.34
	78	N	PRO A	11	46.305	5.494	2.124	1.00 1.00	26.78
15	79	CD	PRO A	11	45.988	6.856	1.655	1.00	9.37 13.93
	80	CA	PRO A	11	45.313	5.030	3.102	1.00	18.39
	81	CB	PRO A	11	44.263	6.137	3.082	1.00	26.39
	82 83	CG C	PRO A	11	45.107	7.388	2.763	1.00	26.16
20	84	ŏ	PRO A PRO A	11	44.718	3.662	2.745	1.00	29.16
20	85	Ň	PRO A	11 12	44.619 44.277	3.300	1.579	1.00	42.47
	86	ČD	PRO A	12	44.139	2.911 3.482	3.759	1.00	29.44
	87	CA	PRO A	12	43.673	1.578	5.107 3.725	1.00	42.51
~ -	88	CB	PRO A	12	43.049	1.454	5.115	1.00 1.00	43.05 41.74
25	89	CG	PRO A	12	43.957	2.251	5.951	1.00	59.93
	90	C	PRO A	12	42.625	1.358	2.645	1.00	51.72
	91	0	PRO A	12	42.384	0.223	2.220	1.00	61.36
	92 93	N CA	TRP A TRP A	13	41.985	2.444	2.231	1.00	52.05
30	94	CB	TRP A	13	40.926	2.405	1.232	1.00	45.67
-	95	CG	TRP A	13 13	40.423	3.818	1.033	1.00	48.38
	96	CD2	TRP A	13	40.354 39.731	4.497 3.991	2.343	1.00	49.00
	97	CE2	TRP A	13	39.943	4.934	3.519 4.542	1.00 1.00	33.76
	98	CE3	TRP A	13	39.013	2.827	3.809	1.00	31.11
35	99	CD1	TRP A	13	40.908	5.693	2.685	1.00	30.50 46.06
	100	NE1	TRP A	13	40.667	5.962	4.005	1.00	48.28
	101	CZ2	TRP A	13	39.463	4.755	5.837	1.00	28.30
	102 103	CZ3 CH2	TRP A	13	38.536	2.646	5.102	1.00	40.23
40	103	C	TRP A	13	38.764	3.610	6.100	1.00	32.97
	105	ŏ	TRP A	13 13	41.348	1.802	-0.087	1.00	47.41
	106	Ň	ASN A	14	42.162 40.796	2.382 0.627	-0.809	1.00	45.41
	107	CA	ASN A	14	41.102	-0.084	-0.386 -1.622	1.00 1.00	52.08
4	108	CB	ASN A	14	40.891	-1.578	-1.434	1.00	50.75 45.92
45	109	CG	ASN A	14	39.442	-1.920	-1.257	1.00	58.48
	110	OD1	ASN A	14	38.790	-1.435	-0.331	1.00	59.48
	111 112	ND2 C	ASN A	14	38.916	-2.747	-2.153	1.00	60.88
	113	ŏ	ASN A ASN A	14	40.171	0.433	-2.716	1.00	49.24
50	114	Ň	ARG A	15	40.280 39.238	0.060	-3.881	1.00	55.28
	115	CA	ARG A	15	38.310	1.284 1.895	-2.317	1.00	40.77
	116	CB	ARG A	15	36.875	1.556	-3.250 -2.879	1.00 1.00	33.20
	117	CG	ARG A	15	36.724	0.305	-2.085	1.00	21.25
55	118	CD	ARG A	15	35.250	0.125	-1.761	1.00	42.18 35.91
55	119	NE	ARG A	15	34.488	-0.087	-2.981	1.00	10.90
	120 121	CZ NH1	ARG A	15	33.194	0.157	-3.092	1.00	35.38
	122	NH2	ARG A ARG A	15	32.538	0.624	-2.051	1.00	33.36
	123	C	ARG A	15 15	32.563	-0.078	-4.231	1.00	59.41
60	124	ŏ	ARG A	15	38.518 38.262	3.406 3.995	-3.108	1.00	32.71
	125	N	ILE A	16	38.965	4.051	-2.058 -4.168	1.00	18.86
	126	CA	ILE A	16	39.191	5.470	-4.083	1.00 1.00	25.83 22.32
	127	CB	ILE A	16	40.666	5.698	-4.000	1.00	4.67
65	128	CG2	ILE A	16	41.229	4.810	-2.957	1.00	24.87
05	129	CG1	ILE A	16	41.319	5.326	-5.326	1.00	5.49
•	130 131	CD1	ILE A	16	42.840	5.449	-5.311	1.00	5.72
	132	C	ILE A ILE A	16	38.620	6.262	-5.253	1.00	27.38
	133	Ň	PHE A	16 17	38.407	5.729 7.545	-6.332	1.00	50.75
70	134	CA	PHE A	17	38.380 37.877	7.545 8.447	-5.024	1.00	29.15
			• •			•	-6.047	1.00	14.06

	135 136	CB CG	PHE A	17.	37.408	9.741	-5.400	1.00	10.31
	137	CD1	PHE A PHE A	17 17	36.041	9.655	-4.819	1.00	5.03
	138	CD2	PHE A	17	35.697 35.071	10.396 8.885	-3.697	1.00	17.85
5	139	CE1	PHE A	17	34.385	10.376	-5.431 -3.190	1.00	6.30
	140	CE2	PHE A	17	33.743	8.853	-4.934	1.00 1.00	28.74
	141	CZ	PHE A	17	33.399	9.598	-3.817	1.00	28.88 19.77
	142	С	PHE A	17	38.975	8.769	-7.051	1.00	25.28
10	143	0	PHE A	17	40.159	8.770	-6.717	1.00	27.78
10	144	N	LYS A	18	38.567	9.041	-8.283	1.00	38.02
	145	CA	LYS A	18	39.502	9.379	-9.34 6	1.00	41.11
	146 147	CB CG	LYS A LYS A	18	38.736	9.665	-10.645	1.00	37.45
	148	CD	LYS A LYS A	18 18	39.565 38.672	10.297	-11.754	1.00	38.42
15	149	CE	LYS A	18	38.672 39.477	10.698 11.290	-12.919	1.00	71.68
••	150	NZ	LYS A	18	40.148	12.572	-14.078 -13.720	1.00	82.18
	151	C	LYS A	18	40.280	10.612	-8.932	1.00 1.00	90.91
	152	0	LYS A	18	39.707	11.549	-8.376	1.00	42.58 50.79
00	153	N	GLY A	19-	41.582	10.607	-9.193	1.00	38.08
20	154	ÇA	GLY A	19	42.389	11.763	-8.843	1.00	50.88
	155	Ç	GLY A	19	42.987	11.754	-7.445	1.00	51.07
	156	0	GLY A	19	43.838	12.600	-7.117	1.00	53.98
	157 158	N CA	GLU A	20	42.537	10.820	-6.609	1.00	35.00
25	159	CB	GLU A GLU A	20 20	43.081	10.712	-5.266	1.00	30.62
	160	CG	GLU A	20	42.113 40.753	9.993	-4.338	1.00	17.69
	161	CD	GLU A	20	39.951	10.651 . 10.197	-4.261	1.00	52.43
	162	OE1	GLU A	20	39.832	8.970	-3.050 -2.842	1.00	59.33
	163	OE2	GLU A	20	39.437	11.064	-2.306	1.00 1.00	67.80
30	164	С	GLU A	20	44.402	9.953	-5.301	1.00	52.52 40.13
	165	0	GLU A	20	44.789	9.367	-6.321	1.00	29.35
	166	N	ASN A	21	45.089	9.958	-4.171	1.00	39.02
	167	CA	ASN A	21	46.375	9.303	-4.083	1.00	35.97
35	168 169	CB	ASN A	21	47.390	10.310	-3.549	1.00	52.23
55	170	CG OD1	ASN A ASN A	21	47.721	11.379	-4.569	1.00	60.60
	171	ND2	ASN A	21 21	48.190 47.493	11.032	-5.657	1.00	71.53
	172	C	ASN A	21	46.307	12.658 8.066	-4.253 -3.204	1.00	51.64
	173	Ō	ASN A	21	45.377	7.916	-2.390	1.00 1.00	39.75
40	174	N	VAL A	22	47.263	7.160	-3.393	1.00	35.49 30.65
	175	CA	VAL. A	22	47.311	5.934	-2.597	1.00	25.06
	176	CB	VAL A	22	46.241	4.918	-3.040	1.00	31.80
	177	CG1	VAL A	22	46.606	4.337	-4.418	1.00	36.39
45	178 179	CG2	VAL A	22	46.083	3.825	-1.985	1.00	5.71
73	180	C O	VAL A VAL A	22	48.678	5.312	-2.761	1.00	33.39
	181	Ň	THR A	22 23	49.291 49.168	5.422	-3.833	1.00	34.28
	182	ĊA	THR A	23	50.499	4.669 4.073	-1.704 -1.755	1.00	44.00
	183	CB	THR A	23	51.497	4.815	-1.755 -0.829	1.00 1.00	47.12
50	184	OG1	THR A	23	51.516	6.216	-1.138	1.00	48.39 51.20
	185	CG2	THR A	23	52.903	4.243	-1.015	1.00	33.54
	186	Ç	THR A	23	50.508	2.610	-1.356	1.00	39.06
	187	0	THR A	23	50.146	2.261	-0.228	1.00	40.82
55	188 189	N CA	LEU A	24	50.920	1.758	-2.286	1.00	36.12
JJ	190	CA CB	LEU A LEU A	24	50.982	0.337	-2.012	1.00	42.23
	191	čĠ	LEU A	24 24	50.773 49.429	-0.471	-3.294	1.00	36.69
	192	CD1	LEU A	24	49.240	-0.222 -1.186	-3.968 -5.117	1.00	33.10
	193	CD2	LEU A	24	48.321	-0.391	-5.117 -2.938	1.00 1.00	50.66
60	194	С	LEU A	24	52.352	0.044	-1.444	1.00	31.21 42.69
	195	0	LEU A	24	53.364	0.492	-1.991	1.00	30.60
	196	N	THR A	25	52.392	-0.704	-0.346	1.00	52.44
	197	· CA	THR A	25	53.667	-1.046	0.263	1.00	58.07
65	198 199	CB	THR A	25	53.806	-0.422	1.652	1.00	62.06
J	200	OG1 CG2	THR A	25	53.423	0.958	1.601	1.00	59.04
	201	C	THR A THR A	25 25	55.252	-0.519	2.115	1.00	57.89
	202	ŏ	THR A	25 25	53.820 52.874	-2.557 -3.261	0.373	1.00	58.45
	203	Ň	CYS A	26	55.015	-3.261 -3.039	0.754 0.035	1.00	57.55
70	204	CA	CYS A	26	55.334	-4.465	0.035	1.00 1.00	48.91
							J.001	1.00	53.25

	205	C	CYS A	26	56.187	-4.793	1.272	1.00	65.04
	206	0	CYS A	26	57.370	-4.444	1.305	1.00	65.21
	207	CB:	CYS A	26	56.103	-4.833	-1.201	1.00	62.05
_	208	SG '	CYS A	26	56.163	-6.602	-1.640	1.00	58.57
5	209	N	ASN A	27	55.594	-5.489	2.266		76.24
	210	CA	ASN A	27	56.319	-5.806	3.490	1.00	76.22
	211	СВ	ASN A	27	55.742	-5.025	4.670	1.00	94.33
	212	CG	ASN A	27	54.369	-5.518	5.080	1.00	99.45
	213	OD1	ASN A	27	53.835	-6.457	4.490	1.00	114.67
10	214	ND2	ASN A	27	53.792	-4.886		1.00	126.31
	215	C	ASN A	27	56.288	-7.302	6.095	1.00	113.87
	216	ŏ	ASN A	27	55.477		3.775	1.00	96.08
	217	Ň	GLY A	28	57.227	-8.061	3.274	1.00	101.25
	218	CA	GLY A			-7.729	4.653	1.00	92.99
15	219	Č		28	57.316	-9.125	5.042	1.00	93.67
13	220	ŏ	GLY A	28	58.420	-9.329	6.058	1.00	97.85
	221	N	GLY A	28	59.153	-8.393	6.368	1.00	107.57
	222	CA	ASN A	29	58.544	-10.542	6.583	1.00	96.86
	223		ASN A	29	59.581	-10.846	7.561	1.00	94.84
20	224	CB	ASN A	29	59.517	12.310	7.954	1.00	99.10
20		CG	ASN A	29	58.106	-12.811	8.040	1.00	116.98
	225	OD1	ASN A	29	57.352	-12.453	8.948	1.00	116.13
	226	ND2	ASN A	29	57.726	-13.631	7.077	1.00	132.36
	227	C	ASN A	29	60.941	-10.562	6.954	1.00	97.30
25	228	0	ASN A	29	61.245	-11.011	5.846	1.00	100.89
23	229	N	ASN A	30	61.761	-9 .821	7.683	1.00	95.34
	230	CA	ASN A	30	63.090	-9.479	7.209	1.00	100.29
	231	CB	ASN A	30	63.751	-8.483	8.165	1.00	108.20
	232	CG	ASN A	30	62.971	-7.188	8.288	1.00	117.57
20	233	OD1	ASN A	30	62.798	-6.453	7.314	1.00	118.50
30	234	ND2	ASN A	30	62.494	-6.900	9.498	1.00	125.45
	235	С	ASN A	30	63.979	-10.709	7.086	1.00	99.61
	236	0	ASN A	30	65.174	-10.573	6.812	1.00	111.39
	237	N	PHE A	31	63.407	-11.903	7.278	1.00	87.84
~~	238	CA	PHE A	31	64.181	-13.146	7.201	1.00	71.61
35	239	CB	PHE A	31	63.288	-14.344	6.949	1.00	63.53
	240	CG	PHE A	31	63.993	-15.645	7.148	1.00	71.95
	241	CD1	PHE A	31	64.017	-16.257	8.395	1.00	
	242	CD2	PHE A	31	64.687	-16.234	6.099	1.00	79.52
	243	CE1	PHE A	31	64.724	-17.444	8.595	1.00	82.44 77.29
40	244	CE2	PHE A	31	65.400	-17.420	6.284	1.00	
	245	CZ	PHE A	31	65.420	-18.025	7.538	1.00	89.06
	246	С	PHE A	31	65.252	-13.102	6.111	1.00	83.28
	247	0	PHE A	31	66.452	-13.207	6.393	1.00	69.17
	248	N	PHE A	32	64.809	-12.971	4.865	1.00	84.06
45	249	CA	PHE A	32	65.736	-12.851	3.750	1.00	59.43
	250	СВ	PHE A	32	65.255	-13.673	2.565	1.00	52.65
	251	CG	PHE A	32	65.585	-15.134	2.659	1.00	41.66
	252	CD1	PHE A	32	64.584	-16.073	2.907		47.56
	253	CD2	PHE A	32	66.897	-15.575	2.492	1.00	44.68
50	254	CE1	PHE A	32	64.883	-17.433		1.00	51.53
	255	CE2	PHE A	32	67.208	-16.938	2.989	1.00	43.51
	256	CZ	PHE A	32	66.196	-17.866	2.580	1.00	51.46
	257	Č	PHE A	32			2.824	1.00	52.70
	258	Ö	PHE A	32	65.794 64.773	-11.375	3.345	1.00	58.83
55	259	N	GLU A	33	66.990	-10.698	3.278	1.00	56.92
	260	CA	GLU A	33	67.152	-10.875	3.080	1.00	62.55
	261	CB	GLU A	33		-9.482	2.695	1.00	69.28
	262	CG	GLU A		68.640	-9.164	2.586	1.00	88.52
	263	· CD	GLU A	33	69.291	-8.758	3.901	1.00	69.46
60	264	OE1	GLU A	33	70.782	-8.585	3.753	1.00	84.74
•	265	OE2		33	71.225	-8.087	2.697	1.00	88.47
	266	C	GLU A GLU A	33	71.516	-8.945	4.693	1.00	105.94
	267	ŏ		33	66.436	-9.106	1.391	1.00	64.49
	268	N	GLU A	33	66.268	-9.936	0.490	1.00	58.36
65			VAL A	34	66.045	-7.837	1.292	1.00	53.30
0 5	269 270	CA	VAL A	34	65.345	-7.329	0.123	1.00	45.11
	270 271	CB	VAL A	34	63.852	-7.116	0.440	1.00	48.71
	271 272	CG1	VAL A	34	63.143	-6.517	-0.760	1.00	64.13
	272	CG2	VAL A	34	63.207	-8.418 °	0.846	1.00	12.46
70	273	C	VAL A	34	65.902	-5. 99 2	-0.379	1.00	53.63
70	274	0	VAL A	34	65.671	-4.944	0.233	1.00	61.37

	275 276	N CA	SER A	35- 35	66.614 67.155	-6.020 -4.790	-1.499 -2.063	1.00 1.00	49.22 59.53
	277	CB:	SER A	35	68.650	-4.931	-2.345	1.00	70.72
_	278	OG ·	SER A	35	68.886	-5.671	-3.532	1.00	78.30
5	279	Ç	SER A	35	66.438	-4.442	-3.362	1.00	65.71
	280	0	SER A	35	66.894	-3.576	-4.106	1.00	79.59
	281 282	N CA	SER A SER A	36 36	65.325	-5.122	-3.631	1.00	71.64
	283	CB	SER A	36 36	64.546 65.307	-4.889 -5.378	-4.849 -6.084	1.00	68.57
10	284	og Og	SER A	36	65.260	-6.790	-6.186	1.00 1.00	72.44
	285	C	SER A	36	63,197	-5.593	-4.805	1.00	79.50 63.12
	286	0	SER A	36	63.070	-6.691	-4.265	1.00	64.24
	287	N	THR A	37	62.189	-4.961	-5.391	1.00	60.88
15	288	CA	THR A	37	60.850	-5.529	-5.417	1.00	47.23
13	289 290	CB OG1	THR A THR A	37 37	59.864	-4.621	-4.687	1.00	45.28
	291	CG2	THR A	37	60.421 58.521	-4.251 -5.336	-3.420 -4.477	1.00	61.45
	292	C	THR A	37	60.363	-5.712	-6.854	1.00 1.00	29.55 48.75
	293	0	THR A	37	60.992	-5.240	-7.809	1.00	46.73 46.94
20	294	N	LYS A	38	59.244	-6.406	-7.002	1.00	44.37
	295	CA	LYS A	38	58.658	-6.655	-8.308	1.00	27.76
	296 297	CB CG	LYS A	38	58.820	-8.117	-8.693	1.00	41.96
	298	CD	LYS A LYS A	38 38	59.620	-8.368 -7.977	-9.929	1.00	34.76
25	299	CE	LYS A	38	61.033 61.944	-7.877 -8.534	-9.768 -10.793	1.00	57.35
	300	NZ	LYS A	38	61.835	-10.029	-10.698	1.00 1.00	65.86 34.19
	301	С	LYS A	38	57.184	-6.351	-8.160	1.00	39.95
	302	0	LYS A	38	56.489	-6.975	-7.341	1.00	37.00
30	303	N	TRP A	39	56.705	-5.384	-8.934	1.00	51.66
30	304 305	CA CB	TRP A	39	55.292	-5.012	-8.878	1.00	46.32
	306	CG	TRP A	39 39	55.130 55.477	-3.498 -3.023	-8.736	1.00	37.04
	307	CD2	TRP A	39	54.615	-3.023	-7.372 -6.233	1.00 1.00	41.46 14.22
	308	CE2	TRP A	39	55.360	-2.534	-5.141	1.00	5.00
35	309	CE3	TRP A	39	53.284	-3.389	-6.025	1.00	27.18
	310	CD1	TRP A	39	56.685	-2.548	-6.940	1.00	38.68
	311	NE1	TRP A	39	56.622	-2.252	-5.597	1.00	29.64
	312 313	CZ2 CZ3	TRP A	39 39	54.819 52.745	-2.396	-3.864	1.00	25.70
40	314	CH2	TRP A	39	52.745 53.514	-3.253 -2.761	-4.742 -3.683	1.00 1.00	38.07 26.72
	315	C	TRP A	39	54.531	-5.501	-10.102	1.00	25.72 35.61
	316	0	TRP A	39	55.080	, -5.587	-11.209	1.00	19.21
	317	N	PHE A	40	53.266	-5.833	-9.898	1.00	11.64
45	318	CA	PHE A	40	52.480	-6.327	-10.994	1.00	6.70
40	319 320	CB CG	PHE A	40 40	52.340	-7.853	-10.899	1.00	19.61
	321	CD1	PHE A	40	53. 6 44 54.445	-8.595 -8.807	-11.029	1.00	22.54
	322	CD2	PHE A	40	54.100	-9.019	-9.935 -12.262	1.00 1.00	38.72 33.22
	323	CE1	PHE A	.40	55.673	-9.409	-10.067	1.00	29.68
50	324	CE2	PHE A	40	55.334	-9.625	-12.395	1.00	36.71
	325	CZ	PHE A	40	56.117	-9.818	-11.296	1.00	35.88
	326 327	C	PHE A	40	51.108	-5.687	-11.031	1.00	37.09
	328	N	PHE A HIS A	40 41	50.263 50.902	-5.931 -4.846	-10.145	1.00	42.94
55	329	ĞA	HIS A	41	49.604	-4.207	-12.046 -12.245	1.00 1.00	41.78
	330	CB	HIS A	41	49.734	-2.831	-12.878	1.00	41.13 45.29
	331	CG	HIS A	41	48.457	-2.055	-12.857	1.00	22.20
	332	CD2	HIS A	41	48.178	-0.784	-13.225	1.00	33.03
60	333 334	ND1	HIS A	41	47.288	-2.576	-12.347	1.00	36.74
UU	335	CE1 NE2	HIS A	41	46.341	-1.656	-12.396	1.00	31.11
	336	C	HIS A HIS A	41 41	46.856 48.903	-0.558 -5.131	-12.924 -13.215	1.00 1.00	55.47
	337	ō	HIS A	41	49.468	-5.495	-14.246	1.00	29.92
	338	Ň	ASN A	42	47.688	-5.532	-12.876	1.00	19.98 26.06
65	339	CA	ASN A	42	46.968	-6.458	-13.730	1.00	33.33
	340	CB	ASN A	42	46.265	-5.680	-14.834	1.00	17.02
	341	CG OD1	ASN A	42	45.045	-4.956	-14.334	1.00	32.02
	342 343	ND2	ASN A ASN A	42 42	44.490	-5.335	-13.274	1.00	29.56
70	344	C	ASN A	42	44.618 47.924	-3.945 -7.520	-15.101 -14.333	1.00	13.43
					77.327	-7.020	-14.333	1.00	38.30

	0.45	•	4014	4-					
	345 346	0 N	ASN A GLY A	42 · 43	47.954 48.723	-7.738 -8.150	-15.548 -13.476	1.00	35.70
	347	CA :	GLY A	43	49.640	-9.182	-13.926	1.00 1.00	39.92 32.70
_	348	C .	GLY A	43	50.880	-8.741	-14.686	1.00	36.33
5	349	0	GLY A	43	51.786	-9.544	-14.891	1.00	40.53
	350 351	N CA	SER A SER A	44 44	50.946 52.124	-7.489 -7.048	-15.117 -15.862	1.00	34.42
	352	CB	SER A	44	51.738	-6.0 5 5	-16.957	1.00 1.00	44.42 57.35
	353	OG	SER A	44	50.928	-6.677	-17.942	1.00	77.66
10	354	C	SER A	44	53.128	-6.402	-14.947	1.00	42.83
	355 356	0 N	SER A LEU A	44 45	52.755	-5.629	-14.072	1.00	48.20
	357	CA	LEU A	45 45	54.404 55.472	-6.713 -6.160	-15.153 -14.322	1.00 1.00	46.97
	358	СВ	LEU A	45	56.819	-6.805	-14.665	1.00	46.50 33.26
15	359	CG	LEU A	45	58.045	-6.173	-13.999	1.00	34.18
	360	CD1	LEU A	45	57.912	-6.233	-12.476	1.00	58.24
	361 362	CD2 C	LEU A LEU A	45 45	59.287 55.581	-6.896 -4.658	-14.445 -14.501	1.00	39.00
	363	ŏ	LEU A	45	55.627	-4 .180	-15.611	1.00 1.00	46.94 34.79
20	364	N	SER A	46	55.612	-3.922	-13.400	1.00	60.24
	365	CA	SER A	46	55.721	-2.478	-13.456	1.00	54.99
	366 367	CB OG	SER A SER A	46 46	55.040 55.175	-1.857 -0.446	-12.240 -12.254	1.00	58.08
	368	č	SER A	46	57.191	-2.132	-13.442	1.00 1.00	81.72 58.15
25	369	0	SER A	46	58.023	-2.965	-13.100	1.00	70.14
	370	N	GLU A	47	57.513	-0.902	-13.819	1.00	57.45
	371 372	CA CB	GLU A GLU A	47 47	58.900 59.070	-0.462 0.748	-13.822	1.00	65.18
	373	CG	GLU A	47	58.981	0.748 0.417	-14. 73 5 -16.207	1.00 1.00	75.20 98.71
30	374	CD	GLU A	47	59.119	1.648	-17.075	1.00	118.62
	375	OE1	GLU A	47	58.207	2.505	-17.038	1.00	131.08
	376 377	OE2 C	GLU A GLU A	47 47	60.140	1.761	-17.788	1.00	126.76
	378	ŏ	GLU A	47	59.352 60.551	-0.109 -0.117	-12.408 -12.108	1.00 1.00	63.59 67.24
35	379	N	GLU A	48	58.382	0.193	-11.546	1.00	53.32
	380	CA	GLU A	48	58.653	0.539	-10.156	1.00	55.75
	381 382	CB CG	GLU A	48	57.343	0.802	-9.422	1.00	58.11
	383	CD	GLU A	48 48	57.530 58.235	1.166 2.501	-7.964 -7.781	1.00 1.00	86.91 104.21
40	384	OE1	GLU A	48	57.545	3.548	-7.752	1.00	116.45
	385	OE2	GLU A	48	59.483	2.499	-7.681	1.00	107.36
	386 387	C	GLU A GLU A	48	59.403	-0.581	-9.442	1.00	57.10
	388	Ň	THR A	48 49	59.016 60.471	-1.744 -0.230	-9.518 -8.735	1.00 1.00	64.00
45	389	CA	THR A	49	61.253	-1.238	-8.024	1.00	54.72 63.14
	390	CB	THR A	49	62.646	-1.380	-8.647	1.00	63.41
	391 392	OG1 CG2	THR A	49	62.980	-0.174	-9.345	1.00	62.51
	393	C	THR A THR A	49 49	62.677 61.415	-2.552 -1.015	-9.603 -6.521	1.00	64.13
50	394	ŏ	THR A	49	62.066	-1.806	-5.839	1.00 1.00	62.86 69.10
	395	N	ASN A	50	60.821	0.052	-6.003	1.00	54.53
	396 307	CA	ASN A	50	60.918	0.341	-4.580	1.00	61.75
	397 398	CB CG	ASN A ASN A	50 50	60.864 61.974	1.860 2.623	-4.331 E 065	1.00	76.64
55	399	OD1	ASN A	50	63.136	2.211	-5.065 -5.063	1.00 1.00	80.85 73.80
	400	ND2	SN A	50	61.615	3.745	-5.686	1.00	83.17
	401	C	ASN A	50	59.795	-0.365	-3.827	1.00	60.45
	402 403	0 N	ASN A SER A	50 51	58.718 60.053	-0.579 -0.723	-4.361	1.00	64.31
60	404	CA	SER A	51	59.067	-1.417	-2.579 -1.767	1.00 1.00	64.42 69.19
	405	СВ	SER A	51	59.649	-1.690	-0.383	1.00	83.18
	406 407	oe	SER A	51	60.136	-0.498	0.207	1.00	98.67
	407 408	C	SER A SER A	51 51	57.757 56.779	-0.651 -1.160	-1.633	1.00	72.43
65	409	Ň	SER A	51 52	56.779 57.738	-1.160 0.577	-1.076 -2.138	1.00 1.00	75.57 72.75
	410	CA	SER A	52	56.535	1.391	-2.069	1.00	72.75
	411	CB	SER A	52	56.766	2.600	-1.165	1.00	77.27
	412 413	OG C	SER A	52 52	57.143	2.182	0.137	1.00	104.21
70	414	ŏ	SER A SER A	52 52	56.106 56.806	1.858 2.617	-3.449 -4.114	1.00	69.39
	-	-			JJ.500	E	-7.11 4	1.00	68.69

	415	N	LEU A	53 ⁻	54.950	1.376	-3.883	1.00	70.92
	416	CA	LEU A	53	54.405	1.754	-5.176	1.00	66.04
•	417 418	CB ·	LEU A	53	53.747	0.542	-5.841	1.00	64.62
5	419	CD1	LEU A LEU A	53 53	52.954	0.809	-7.120	1.00	57.82
9	420	CD2	LEU A	53 53	53.761	1.661	-8.068	1.00	53.42
	421	C	LEU A	53	52.593 53.383	-0.504 2.879	-7.758	1.00	52.64
	422	ō	LEU A	53	52.319	2.688	-4.975 -4.348	1.00	58.35
	423	N	ASN A	54	53.708	4.055	-5.500	1.00	38.80
10	424	CA	ASN A	54	52.820	5.195	-5.344	1.00 1.00	47.61
	425	CB	ASN A	54	53.638	6.453	-5.089	1.00	60.77 62.70
	426	CG	ASN A	54	54.433	6.376	-3.804	1.00	72.45
	427	OD1	ASN A	54	53.865	6.317	-2.708	1.00	70.70
15	428	ND2	ASN A	54	55.761	6.373	-3.927	1.00	70.84
13	429 430	C O	ASN A	54	51.905	5.420	-6.534	1.00	55.42
	431	N	ASN A ILE A	54 55	52.308	5.246	-7.678	1.00	52.22
	432	ČA	ILE A	55 55	50.669	5.807	-6.241	1.00	47.52
	433	CB	ILE A	55	49.681 48.459	6.089 5.177	-7.267	1.00	48.77
20	434	CG2	ILE A	55	47.338	5.670	-7.138 -8.055	1.00 1.00	48.20
	435	CG1	ILE A	55	48.848	3.746	-7.493	1.00	64.85 17.58
	436	CD1	ILE A	55	47.667	2.811	-7.511	1.00	22.96
	437	Č	ILE A	55	49.242	7.528	-7.070	1.00	53.16
25	438	0	ILE A	55	48.602	7.862	-6.062	1.00	50.16
23	439 440	N CA	VAL A	56	49.576	8.374	-8.041	1.00	53.12
	441	CB	VAL A VAL A	56 50	49.200	9.784	-7.939	1.00	55.98
	442	CG1	VAL A	56 56	50.475	10.660	-8.216	1.00	53.06
	443	CG2	VAL A	56	50.160 51.656	12.096 10.181	-7.893 7.893	1.00	67.53
30	444	Č.	VAL A	56	48.109	10.161	-7.396	1.00	38.93
	445	0	VAL A	56	48.152	9.979	-8.867 -10.075	1.00 1.00	54.49
	446	N	ASN A	57	47.094	10.850	-8.287	1.00	42.98 63.99
	447	CA	ASN A	57	45.941	11.323	-9.041	1.00	72.29
35	448	CB	ASN A	57	46.339	12.495	-9.945	1.00	88.41
33	449 450	CG	ASN A	57	46.916	13.667	-9.157	1.00	95.72
•	450 451	OD1 ND2	ASN A	57	46.274	14.182	-8.236	1.00	90.65
	452	C	ASN A ASN A	57 57	48.133	14.089	-9.512	1.00	90.43
	453	ŏ	ASN A	57	45.413 45.349	10.169 10.232	-9.866	1.00	67.43
40	454	Ň	ALA A	58	45.04 6	9.107	-11.089 <i>-</i> 9.161	1.00	76.76
	455	, CA	ALA A	58	44.526	7.893	-9.764	1.00 1.00	65.44 59.50
	456	CB	ALA A	58	43.813	7.065	-8.715	1.00	51.61
	457	C	ALA A	58	43.591	8.128	-10.925	1.00	56.95
45	458	0	ALA A	58	42.696	8.976	-10.860	1.00	59.56
45	459 460	N CA	LYS A	59	43.815	7.356	-11.984	1.00	54.03
	481	CB	LYS A LYS A	59 50	42.999	7.392	-13.188	1.00	56.80
	462	CG	LYS A	59 59	43.897	7.371	-14.432	1.00	52.13
	463	CD	LYS A	59	44.932 46.010	8.485 8.238	-14.454 15.500	1.00	75.19
50	464	CE	LYS A	59	47.122	9.272	-15.500 -15.379	1.00 1.00	87.07
	465	NZ	LYS A	59	48.271	8.958	-16.271	1.00	101.21 106.25
	466	Č	LYS A	59	42.171	6.106	-13.095	1.00	51.59
	467	0	LYS A	59	42.354	5.318	-12.167	1.00	37.92
55	468	N CA	PHE A	60	41.241	5.888	-14.015	1.00	54.25
<i>JJ</i>	469 470	CA CB	PHE A	60	40.470	4.657	-13.946	1.00	48.76
	471	CG	PHE A	60 60	39.250	4.729	-14.854	1.00	54.70
	472	CD1	PHE A	60	38.304 38.495	5.832	-14.506	1.00	37.20
	473	CD2	PHE A	60	37.215	7.117 5.583	-15.002 -13.694	1.00	29.43
60	474	CE1	PHE A	60	37.606	8.134	-13.684 -14.687	1.00 1.00	37.72
	475	CE2	PHE A	60	36.315	6.597	-13.358	1.00	40.04 23.38
	476	cz	PHE A	60	36.510	7.875	-13.860	1.00	30.49
	477	Ç	PHE A	60	41.388	3.529	-14.397	1.00	45.95
65	478 470	0	PHE A	60	41.263	2.389	-13.957	1.00	37.39
O)	479 480	N CA	GLU A	61	42.326	3.865	-15.276	1.00	48.08
	481	CA CB	GLU A GLU A	61	43.279	2.887	-15.782	1.00	61.34
	482	CG	GLU A	61 61	44.195	3.525	-16.842	1.00	72.31
	483	CD	GLU A	61	43.508 42.606	3.900 5.137	-18.170 18.061	1.00	91.97
70	484	OE1	GLU A	61	43.123	5.127 6.227	-18.061 -17.758	1.00	102.49
			,,			U.E.E.I	-17.758	1.00	100.34

	485 486	OE2 C	GLU A GLU A	61 - 61	41.381 44.116	4.993 2.335	-18.283 -14.625	1.00 1.00	100.98
	487	0	GLU A	61	44.781	1.306	-14.754	1.00	57.54
_	488	N	ASP A	62	44.078	3.027	-13.493	1.00	53.72 48.67
5	489	CA	ASP A	62	44.837	2.597	-12.330	1.00	40.78
	490 491	CB	ASP A	62	45.141	3.784	-11.407	1.00	58.38
	491	OD1	ASP A ASP A	62	46.284	4.654	-11.920	1.00	55.63
	493	OD2	ASP A	62 62	47.343	4.090	-12.281	1.00	50.67
10	494	C	ASP A	62	46.122 44.104	5.898 1.519	-11,947	1.00	65.51
	495	Ö	ASP A	62	44.699	0.839	-11.547 -10.711	1.00 1.00	32.95
	496	N	SER A	63	42.808	1.374	-11.800	1.00	33.25 27.08
	497	CA	SER A	63	42.038	0.346	-11.111	1.00	24.76
15	498	CB	SER A	63	40.574	0.381	-11.542	1.00	32.81
15	499	og	SER A	63	39.976	1.632	-11.254	1.00	57.02
	500 501	C	SER A	63	42.639	-1.002	-11.500	1.00	36.75
	502	N	SER A GLY A	63	43.468	-1.094	-12.419	1.00	31.64
	503	CA	GLY A	64 64	42.236 42.790	-2.057	-10.809	1.00	34.81
20	504	Č.	GLY A	64	43.349	-3.348 -4.182	-11.160	1.00	42.02
	505	Ŏ	GLY A	64	43.011	4.005	-10.021 -8.850	1.00 1.00	50.47
	506	N	GLU A	65	44.224	-5.107	-10.387	1.00	48.47 51.85
	507	CA	GLU A	65	44.836	-6.021	-9.436	1.00	43.33
25	508	CB	GLU A	65	44.691	-7.448	-9.953	1.00	52.77
25	509	cg	GLU A	65	45.405	-8.502	-9.135	1.00	52.38
	510	CD OF1	GLU A	65	45.636	-9.792	-9.907	1.00	58.39
	511 512	OE1 OE2	GLU A GLU A	65 65	46.528	-9.798	-10.801	1.00	43.40
	513	C	GLU A	65 65	44.917	-10.782	·9.610	1.00	51.74
30	514	ŏ	GLU A	65	46.309 47.057	-5.711 -5.550	-9.240	1.00	45.24
	515	Ň	TYR A	66	46.726	-5.644	-10.212 -7.981	1.00 1.00	39.10
	516	CA	TYR A	66	48.119	-5.363	-7.664	1.00	40.60 35.48
	517	CB	TYR A	66	48.259	-4.029	-6.936	1.00	18.93
35	518	CG	TYR A	66	48.056	-2.817	-7.810	1.00	24.42
22	519	CD1	TYR A	66	46.801	-2.218	·7.927	1.00	27.62
	520 521	CE1 CD2	TYR A TYR A	66	46.618	-1.068	-8.707	1.00	20.61
	522	CE2	TYR A	66 66	49.131 48.968	-2.240 -1.093	-8.493	1.00	20.62
	523	cz	TYR A	66	47.708	-0.506	-9.268 -9.375	1.00	19.14
40	524	OH	TYR A	66	47.546	0.631	-10.149	1.00 1.00	37.26 20.86
	525	С	TYR A	66	48.692	-6.454	-6.789	1.00	20.86 35.81
	526	0	TYR A	66	47.992	-6.973	-5.888	1.00	26.54
	527	N	LYS A	67	49.950	-6.803	-7.071	1.00	20.27
45	528 520	CA	LYS A	67	50.672	-7.827	-6.316	1.00	42.77
77	529 530	CB CG	LYS A Lys a	67 67	50.277	-9.255	-6.735	1.00	42.46
	531	CD	LYS A	67 67	50.131 49.867	-9.502	-8.223	1.00	70.28
	532	ČĒ	LYS A	67	49.313	-10.987 -11.233	-8.489 -9.888	1.00	66.50
	533	NZ	LYS A	67	49.387	-12.668	-10.255	1.00 1.00	73.20
50	534	С	LYS A	67	52.161	-7.648	-6.480	1.00	55.01 49.35
	535	0	LYS A	67	52.656	-7.502	-7.596	1.00	49.27
	536	N	CYS A	68	52.872	-7.632	-5.359	1.00	55.09
	537	CA	CYS A	68	54.314	-7.450	-5.384	1.00	54.74
55	538 539	CO	CYS A	68	54.966	-8.793	-5.171	1.00	42.46
<i>JJ</i>	540	СВ	CYS A CYS A	68 68	54.285	-9.748	-4.779	1.00	18.20
	541	ŠĠ	CYS A	68	54.750 54.393	-6.451 -6.915	-4.309	1.00	64.47
	542	N	GLN A	69	56.267	-8.876	-2.586 -5.444	1.00 1.00	100.38 26.58
	543	CA	GLN A	69	56.968	-10.142	-5.299	1.00	26.57
60	544	CB	GLN A	69	56.693	-10.973	-6.556	1.00	15.18
	545	ÇG	GLN A	69	57.877	-11.704	-7.156	1.00	38.54
	546 547	CD	GLN A	69	57.573	-12.192	-8.567	1.00	36.61
	547 548	OE1	GLN A	69	56.511	-12.787	-8.816	1.00	18.42
65	548 549	NE2 C	GLN A	69 60	58.497	-11.941	-9.498	1.00	36.58
55	550	ŏ	GLN A GLN A	69 69	58.472 50.174	-10.000	-5.034	1.00	41.83
	551	Ň	HIS A	70	59.174 58.951	-9.343 -10.602	-5.804 -3.038	1.00	24.51
	552	CA	HIS A	70	60.375	-10.552	-3.938 -3.568	1.00 1.00	59.31
 -	553	СВ	HIS A	70	60.550	-10.461	-2.050	1.00	54.15 49.67
70	554	ca	HIS A	70	60.025	-9.194	-1.451	1.00	57.18
									- · · · •

	555 556	CD2 ND1	HIS A HIS A	70- 70	59.202 60.376	-8.984 -7.946	-0.397 -1.918	1.00 1.00	57.85
	557	CE1	HIS A	70	59.796	-7.021	-1.178	1.00	60.44 62.11
_	558	NE2	'HIS A	70	59.078	-7.624	-0.246	1.00	69.17
5	559	С	HIS A	70	61.065	-11.814	-4.055	1.00	45.74
	560	0	HIS A	70	60.390	-12.760	-4.466	1.00	48.46
	561	N	GLN A	71	62.397	-11.824	-4.020	1.00	34.41
	562	CA	GLN A	71	63.170	-12.998	-4.434	1.00	34.74
10	563	CB	GLN A	71	64.631	-12.609	-4.631	1.00	28.64
10	564 565	CG CD	GLN A	71	65.521	-13.746	-5.061	1.00	28.58
	566	OE1	GLN A GLN A	71 71	67.021 67.508	-13.427	-4.933	1.00	44.36
	567	NE2	GLN A	71	67.749	-12.432 -14.289	-5.447 -4.?46	1.00	24.64
	568	C	GLN A	71	63.098	-14.123	-3.76	1.00 1.00	82.76
15	569	ō	GLN A	71	63.036	-13.876	-2.168	1.00	42.41 58.78
	570	N	GLN A	72	63.116	-15.369	-3.522	1.00	36.65
	571	CA	GLN A	72	63.062	-16.493	-2.873	1.00	56.26
	572	CB	GLN A	72	64.225	-16.440	-1.894	1.00	66.55
20	573 574	ca	GLN A	72	65.522	-16 962	-2.419	1.00	74.96
20	574 575	CD OE1	GLN A GLN A	72	66.614	-10.771	-1.409	1.00	81.18
	576	NE2	GLN A	72 72	66.932 67.196	-15.625 -17.886	-1.027	1.00	46.66
	577	C	GLN A	72	61.791	-16.614	-0.944 -2.044	1.00 1.00	86.79
	578	ŏ	GLN A	72	61.763	-17.296	-1.035	1.00	47.57 53.55
25	579	N	VAL A	73	60.740	-15.937	-2.457	1.00	25.14
	580	CA	VAL A	73	59.499	-16.027	-1.737	1.00	27.76
	581	СВ	VAL A	73	59.434	14.865	-0.770	1.00	24.20
	582	CG1	VAL A	73	58.034	-14.638	-0.284	1.00	61.77
30	583 584	CG2	VAL A	73	60.349	-15.143	0.383	1.00	48.95
50	585	C O	VAL A VAL A	73 73	58.330	-16.018 -15.385	-2.730	1.00	38.97
	586	Ň	ASN A	73 74	58.405 57.261	-15.385 -16. 73 5	-3.793 -2.392	1.00 1.00	50.48
	587	CA	ASN A	74	56.080	-16.794	-3.251	1.00	30.12 54.75
	588	СВ	ASN A	74	55.023	-17.677	-2.576	1.00	65.77
35	589	CG	ASN A	74	55.444	-19.138	-2.523	1.00	77.30
	590	OD1	ASN A	74	55.408	-19.840	-3.538	1.00	66.94
	591	ND2	ASN A	74	55.871	-19.586	-1.341	1.00	98.68
	592 593	C	ASN A ASN A	74	55.514	-15.392	-3.593	1.00	61.15
40	594	Ň	GLU A	74 75	55. 945 54. 553	14 .38 4 -15 .322	-3.027 -4.523	1.00	65.55
•	595	CA	GLU A	75	53.971	-14.057	-4.951	1.00 1.00	62.19 63.45
	596	CB	GLU A	75	53.296	-14.213	-6.314	1.00	82.08
	597	CG	GLU A	75	54.237	-14.649	-7.425	1.00	101.46
4.5	598	CD	GLU A	75	53.533	-14.804	-8.759	1.00	105.08
45	599	OE1	GLU A	75	52.308	-14.564	-8.815	1.00	85.23
	600	OE2	GLU A	75	54.204	-15.167	-9.747	1.00	113.01
	601 602	C	GLU A GLU A	75 75	52.979	-13.531	-3.920	1.00	46.81
	603	Ň	SER A	75 76	52.180 53.008	-14.279 -12.216	-3.378 -3.667	1.00 1.00	63.28
50	604	CA	SER A	76	52.104	-11.602	-2.698	1.00	44.23 44.01
	605	CB	SER A	76	52.265	-10.080	-2.698	1.00	52.11
	606	OG	SER A	76	51.674	-9.502	-3.854	1.00	49.14
	607	Ç	SER A	76	50.658	-11.942	-3.036	1.00	40.30
55	608	0	SER A	76	50.351	-12.409	-4.122	1.00	37.45
J J	609 610	N	GLU A	77	49.787	-11.733	-2.074	1.00	47.16
	611	CA CB	GLU A GLU A	77 77	48.373	-11.965	-2.345	1.00	50.65
	612	če	GLU A	77 77	47.596 48.051	-12.125 -13.299	-1.037	1.00	64.23
	613	CD	GLU A	77	49.143	-12.917	-0.184 0.795	1.00 1.00	100.08 121.85
60	614	OE1	GLU A	77	49.535	-11.731	0.817	1.00	113.34
	615	OE2	GLU A	77	49.607	-13.804	1.543	1.00	135.86
	616	C	GLU A	77	47.780	-10.837	-3.181	1.00	57.00
	617	0	GLU A	77	48.203	-9.696	-2.996	1.00	70.10
65	618	N	PRO A	78	46.905	-11.147	-4.089	1.00	60.36
UJ	619 620	CD CA	PRO A	78 70	46.349	-12.453	-4.468	1.00	76.75
	621	CB	PRO A PRO A	78 78	46.348	-10.084	-4.915 5.000	1.00	45.94
	622	CG	PRO A	78 78	45.380 45.954	-10.826 -12.210	-5.830 -5.903	1.00	63.85
	623	č	PRO A	78	45.640	-9.054	-5.903 -4.055	1.00 1.00	74.36 46.99
70	624	0	PRO A	78	45.047	-9.380	-3.014	1.00	44.78

	625	N	VAL A	79-	45.723	-7.806	-4.493	1.00	38.75
	626	CA	VAL A	79	45.068	-6.708	-3.808	1.00	46.98
	627	CB:	VAL A	79	46.101	-5.836	-3.067	1.00	48.31
_	628	CG1	VAL A	79	45.700	-4.371	-3.099	1.00	58.66
5	629	CG2	VAL A	79	46.195	-6.289	·1.639	1.00	43.93
	630	C	VAL A	79	44.344	-5.925	-4.907	1.00	41.63
	631	0	VAL A	79	44.974	-5.465	-5.869	1.00	31.43
	632	N	TYR A	80	43.024	-5.799	-4.786	1.00	36.26
10	633	CA	TYR A	80	42.258	-5.105	·5.807	1.00	43.25
10	634 635	CB	TYR A	80	40.986	-5.889	-6.142	1.00	43.58
	636	CG CD1	TYR A	80	41.315	-7.289	-6.619	1.00	62.18
	637	CE1	TYR A TYR A	80	41.297	-8.370	-5.734	1.00	59.18
	638	CD2	TYR A	80	41.695	-9.639	-6.138	1.00	63.70
15	639	CE2	TYR A	80 80	41.738	-7.521	-7.932	1.00	64.60
	640	CZ	TYR A	80	42.141 42.116	-8.793	-8.341	1.00	72.36
	641	OH	TYR A	80	42.116	-9.843 -11.096	-7.439	1.00	71.99
	642	Č.	TYR A	80	41.920	-3.677	-7.848	1.00	86.14
	643	ŏ	TYR A	80	41.299	-3.392	-5.468	1.00	39.91
20	644	N	LEU A	81	42.350	-2.791	-4.445 -6.356	1.00	39.73
	645	CA	LEU A	81	42.130	-1.367	-6.236	1.00	42.49
	646	CB	LEU A	81	43.462	-0.645	·6.434	1.00 1.00	39.83
	647	CG	LEU A	81	43.433	0.870	-6.520	1.00	29.82
	648	CD1	LEU A	81	42.862	1.449	-5.246	1.00	35.37 54.76
25	649	CD2	LEU A	81	44.841	1.363	-6.750	1.00	51.99
	650	С	LEU A	81	41.113	-0.953	-7.307	1.00	40.44
	651	0	LEU A	81	41.218	-1.335	-8.479	1.00	44.23
	652	N	GLU A	82	40.119	-0.175	-6.903	1.00	34.19
20	653	CA	GLU A	82	39.108	0.266	-7.850	1.00	43.16
30	654	СВ	GLU A	82	37.833	-0.540	-7.615	1.00	43.29
	655	CG	GLU A	82	36.683	-0.166	-8.517	1.00	64.74
	656 657	CD	GLU A	82	35.546	-1.157	-8.415	1.00	79.52
	658	OE1 OE2	GLU A	82	35.177	-1.505	-7.272	1.00	89.05
35	659	C	GLU A GLU A	82 82	35.023	-1.586	-9.468	1.00	95.85
-	660	ŏ	GLU A	82	38.802 38.213	1.778	-7.803	1.00	36.44
	661	Ň	VAL A	83	39.200	2.268 2.505	-6.840	1.00	20.88
	662	CA	VAL A	83	38.957	3.947	-8.849 -8.947	1.00	17.32
	663	CB	VAL A	83	39.842	4.587	-10.012	1.00 1.00	20.25 16.19
40	664	CG1	VAL A	83	39.647	6.071	-9.995	1.00	22.13
	665	CG2	VAL A	83	41.280	4.219	-9.786	1.00	30.28
	666	Ç	VAL A	83	37.503	4.274	-9.323	1.00	24.88
	667	0	VAL A	83	36.946	3.744	-10.285	1.00	47.06
45	668	N	PHE A	84	36.894	5.162	-8.555	1.00	14.13
40	669 670	CA CB	PHE A	84	35.520	5.575	-8.800	1.00	26.86
	671	CG	PHE A PHE A	84	34.646	5.374	-7.564	1.00	13.44
	672	CD1	PHE A	84	34.475	3.964	-7.163	1.00	34.33
	673	CD2	PHE A	84	35.571	3.183	-6.840	1.00	45.55
50	674	CE1	PHE A	84 84	33.205 35.405	3.420	-7.070	1.00	44.61
	675	CE2	PHE A	84	33.022	1.865 2.106	-6.433	1.00	65.24
	676	cz	PHE A	84	34.122	1.325	-6.667	1.00	42.90
	677	C	PHE A	84	35.462	7.061	-6.343 -9.146	1.00	65.66
	678	0	PHE A	84	36.490	7.760	·9. i78	1.00 1.00	45.25 38.34
55	679	N	SER A	85	34.234	7.512	-6.399	1.00	48.62
	680	CA	SER .	85	33.919	8.899	-9.712	1.00	37.65
	681	CB	SER A	85	34. 23 2	9.236	-11.159	1.00	40.40
	682	OG.	SER A	85	34.067	10.629	-11.358	1.00	35.89
60	683	Ç	SER A	85	32.438	9.035	-9.467	1.00	22.78
60	684	0	SER A	85	31.630	8.613	-10.264	1.00	37.65
	685	N	ASP A	86	32.098	9.604	-8.326	1.00	14.50
	686	CA	ASP A	86	30.713	9.771	-7.919	1.00	9.43
	687	CB	ASP A	86	30.133	8.405	-7.554	1.00	12.45
65	688 689	CG	ASP A	86	28.611	8.418	-7.427	1.00	51.60
.	690	OD1 OD2	ASP A	86	28.054	9.224	-6.645	1.00	55.89
	691	C	ASP A ASP A	86 86	27.960	7.606	-8.115	1.00	79.60
	692	ŏ	ASP A	86 86	30.746	10.707	-6.680	1.00	28.99
	693	Ň	TRP A	87	31.827 29.583	11.076	-6.199	1.00	31.21
70	694	CA	TRP A	87	29.543	11.104 11.991	-6.171 -5.024	1.00	14.11
		-	**		20.000	11.001	-5.024	1.00	41.60

	695 696	CB CG		A 87			***************************************	1.00	67.93
	697	CD2	TRP				-6.057 -6.312	1.00 1.00	79.67
-	698	CE2	TRP	A 87				1.00	97.15 98.87
5	699	CE3		A 87				1.00	106.42
	700	CD1		A 87				1.00	73.69
	701	NE1	TRP	A 87			-7.994	1.00	66.94
	702 703	CZ2 CZ3	TRP TRP	A 87			-8.083	1.00	111.64
10	704	CH2		A 87				1.00	116.11
	705	C		A 87			-7.392 -3.735	1.00 1.00	119.60
	706	0		A 87			-2.915	1.00	44.35 41.60
	707	N.		A 88			-3.546	1.00	50.46
15	708 70 9	CA CB		A 88			-2.340	1.00	36.94
13	710	CG	LEU	A 88			-1.530	1.00	4.59
	711	ČD1		A 88			-0.861 0.161	1.00	21.69
	712	CD2	LEU				-0.155	1.00 1.00	11.07 21.48
20	713	С	LEU	A 88			-2.655	1.00	28.38
20	714	0	LEU				-3.508	1.00	29.21
	715 716	N CA	LEU				-1.948	1.00	45.92
	717	CB	LEU				-2.092	1.00	35.41
_	718	CG		A 89			-2.623 -2.839	1.00 1.00	12.22
25	719	CD1	LEU				-3.405	1.00	32.05 25.06
	720	CD2		A 89			-3.801	1.00	25.39
	721	C	LEU				-0.721	1.00	21.36
	722 723	0 N		A 89			0.234	1.00	48.70
30	724	CA		A 90			-0.602 0.690	1.00	31.16
	725	CB		A 90			0.796	1.00 1.00	20 <i>.2</i> 7 4.59
	726	CG	LEU				2.145	1.00	5.03
	727	CD1		A 90			3.170	1.00	5.42
35	728 729	CD2 C	LEU	A 90		1.067	2.147	1.00	18.53
	730	ŏ		A 90		3.096 2.129	0. 7 57 0.017	1.00	29.48
	731	N	GLN		34.004		1.612	1.00 1.00	49.50 33.11
	732	CA	GLN		35.308		1.724	1.00	34.25
40	733	CB	GLN		36.389		1.872	1.00	29.25
70	734 735	CD CG	GLN GLN		36.487 37.564		0.664	1.00	4.72
	736	OE1	GLN		37.492		0.795 1.657	1.00 1.00	24.07
	737	NE2	GLN		38.566		-0.075	1.00	33.85 25.90
AE	738	Ç	GLN		35.339		2.892	1.00	39.46
45	739	0	GLN		34.607	2.134	3.875	1.00	41.60
•	·740 741	N CA		A 92			2.774	1.00	33.12
	742	CB		A 92 A 92		-0.064 -1.288	3.844	1.00	44.90
	743	Č		A 92		-0.476	3.498 4.151	1.00 1.00	44.46 45.76
50	744	0		A 92		-0.586	3.253	1.00	51.50
	745	N	SER				5.432	1.00	48.03
	746 747	CA CB	SER SER	A 93		-1.103	5.881	1.00	52.40
	748	OG	SER	A 93 A 93		-1.381 -2.377	7.380	1.00	48.05
55	749	č	SER			-2.364	7.689 5.142	1.00 1.00	47.42
	750	0	SER			-2.593	4.836	1.00	49.91 54.70
	751	N	ALA .			-3.170	4.856	1.00	47.64
	752 753	CA CB	ALA ALA			-4.430	4.161	1.00	40.55
60	754	C	ALA			-5.404 -4.968	5.048	1.00	44.76
	755	Ŏ	ALA .			-5.033	3.823 4.688	1.00 1.00	53.40 40.13
	756	N	GLU .	A 95		-5.347	2.565	1.00	63.75
	757 750	CA	GLU .			-5.865	2.125	1.00	61.37
65	758 759	CB CG	GLU.			-5.940	0.603	1.00	77.66
	760	CD	GLU.			-4.576 -4.640	-0.059 -1.583	1.00	76.66
	761	OE1	GLU			-3.565	-1.582 -2.217	1.00 1.00	9 6 .68 107.34
	762	OE2	GLU .	A 95	36.073	-5.754	-2.151	1.00	107.34
70	763 764	C	GLU			-7.231	2.750	1.00	54.28
, 0	104	0	GLU .	A 95	34.527	-7.667	2.838	1.00	42.98

	765	N	VAL A	96	36.739	-7.903	3.193	1.00	61.87
	766	CA	VAL A	96	36.604	-9.205	3.851	1.00	61.01
	767	CB:	VAL A	96	36.933	-10.354	2.897	1.00	56.77
5	768	CG1	VAL A	96	36.541	-11.670	3.536	1.00	39.60
,	769 770	CG2 C	VAL A	96	36.215	-10.149	1.576	1.00	53.03
	770 771	ŏ	VAL A VAL A	96	37.520	-9.306	5.084	1.00	56.97
	772	Ñ	VAL A VAL A	96	38.751	-9.202	4.985	1.00	45.37
	773	ČA	VAL A	97 07	36.900	-9.512	6.241	1.00	53.01
10	774	CB	VAL A	97 97	37.614	-9.606	7.499	1.00	56.01
	775	CG1	VAL A	97	37.188 37.790	-8.448	8.435	1.00	57.61
	776	CG2	VAL A	97	37.637	-8.628 -7.122	9.802	1.00	87.18
	777	c	VAL A	97	37.372	-10.944	7.858	1.00	68.07
	778	Ŏ	VAL A	97	36.278	-11.542	8.209 8.158	1.00	61.52
15	779	N	MET A	98	38.412	-11.411	8.879	1.00 1.00	38.67
	780	CA	MET A	98	38.335	-12.644	9.633	1.00	64.69 62.72
	781	CB	MET A	98	39.745	-13.081	10.013	1.00	71.28
	782	CG	MET A	98	39.901	-14.561	10.252	1.00	94.38
20	783	SD	MET A	98	39.346	-15.500	8.803	1.00	75.29
20	784	CE	MET A	98	37.821	-16.041	9.448	1.00	93.84
	785	Ç	MET A	98	37.520	-12.336	10.894	1.00	58.92
	786	0	MET A	98	37.748	-11.318	11.552	1.00	61.33
	787	N	GLU A	99	36.573	-13.201	11.241	1.00	61.37
25	788	CA	GLU A	99	35.762	-12.971	12.436	1.00	59.89
23	789	CB	GLU A	99	34.950	-14.211	12.797	1.00	52.02
	790 791	CG	GLU A	99	0 153	-14.039	14.072	1.00	64.75
	791 792	CD OE1	GLU A GLU A	99	33.366	-15.285	14.456	1.00	90.18
	793	OE2	GLU A	99	33.983	-16.375	14.536	1.00	106.04
30	794	C	GLU A	99	32.137	-15.170	14.685	1.00	84.66
50	795	ŏ	GLU A	99 99	36.621	-12.587	13.633	1.00	66.15
	796	Ň	GLU A	100	37.583	-13.284	13.972	1.00	81.55
	797	ĊA	GLY A	100	36.265 37.016	-11.478	14.271	1.00	58.33
	798	č.	GLY A	100	37.943	-11.021 -9.872	15.419	1.00	54.87
35	799	ŏ	GLY A	100	38.293	-9.087	15.088 15.9 6 0	1.00	54.97
	800	N	GLN A	101	38.367	-9.772	13.836	1.00 1.00	69.91
	801	CA	GLN A	101	39.237	-8.671	13.445	1.00	54.17 57.48
	802	CB	GLN A	101	39.942	-8.998	12.125	1.00	60.93
40	803	CG	GLN A	101	41.016	-10.063	12.237	1.00	76.51
40	804	CD	GLN A	101	42.059	-9.719	13.290	1.00	90.62
	805	OE1	GLN A	101	41.825	-9.891	14.490	1.00	100.86
	806	NE2	GLN A	101	43.212	-9.215	12.846	1.00	85.92
	807	C	GLN A	101	38.445	-7.353	13.311	1.00	56.15
45	808	0	GLN A	101	37.210	-7.337	13.344	1.00	44.69
43	809 810	N CD	PRO A	102	39.151	-6.222	13.180	1.00	56.36
	811	CA	PFO A	102	40.600	-5.991	13.326	1.00	60.77
	812	CB	PRO A PRO A	102	38.438	-4.954	13.048	1.00	55.67
	813	CG	PRO A	102 102	39.483	-3.933	13.458	1.00	47.18
50	814	č	PRO A	102	40.742 37.915	-4.538 4.716	12.918	1.00	47.65
	815	ŏ	PRO A	102	38.567	-4.716 5 000	11.631	1.00	58.48
	816	Ň	LEU A	103	36.719	-5.036 -4.151	10.635	1.00	58.71
	817	CA	LEU A	103	36.041	0.000	11.589	1.00	1.34
	818	CB	LEU A	103	34.728	-3.833 -4.610	10.320 10.248	1.00	47.87
55	819	CG	LEU A	103	33.811	4.304	9.073	1.00 1.00	54.63
	820	CD1	LEU A	103	34.546	-4.596	7. 7 67	1.00	54.99
	821	CD2	LEU A	103	32.537	-5.130	9.206	1.00	57.13 49.78
	822	C	LEU A	103	35.761	-2.332	10.359	1.00	39.79
60	823	0	LEU A	103	35.046	-1.847	11.254	1.00	21.76
60	824	N	PHE A	104	36.300	-1.598	9.391	1.00	18.87
	825	CA	PHE A	104	36.111	-0.157	9.393	1.00	30.54
	826	СВ	PHE A	104	37.466	0.500	9.616	1.00	41.57
	827	CG	PHE A	104	37.385	1.948	9.969	1.00	54.55
65	828	CD1	PHE A	104	37.282	2.351	11.301	1.00	72.72
65	829	CD2	PHE A	104	37.441	2.917	8.975	1.00	57.49
	830	CE1	PHE A	104	37.227	3.706	11.640	1.00	70.88
	831	CE2	PHE A	104	37.385	4.273	9.297	1.00	60.17
	832 833	CZ	PHE A	104	37.285	4.670	10.633	1.00	66.74
70	834	C	PHE A	104	35.466	0.437	8.137	1.00	35.62
, 0	007	J	PHE A	104	36.079	0.468	7.066	1.00	37.03

	835	N	LEU A	105	34.234	0.922	8.269	1.00	20.44
	836	CA	LEU A	105	33.541	1.550	7.144	1.00	36.14 48.60
	837	CB	LEU A	105	32.073	1.154	7.125	1.00	46.94
5	838 839	CG.	LEU A	105	31.870	-0.297	6.725	1.00	52.90
,	840	CD1	LEU A	105	30.385	-0.564	6.516	1.00	46.80
	841	CD2 C	LEU A	105	32.663	-0.562	5.442	1.00	53.92
	842	ŏ	LEU A LEU A	105	33.658	3.072	7.195	1.00	46.53
	843	Ň	ARG A	105	33.938	3.645	8.241	1.00	50.68
10	844	CA	ARG A	106 106	33.406 33.539	3.725	6.066	1.00	45.66
	845	CB	ARG A	106	35.021	5.172	5.962	1.00	26.49
	846	ĊĠ	ARG A	106	35.354	5.513 6.951	5.786	1.00	36.08
	847	CD	ARG A	106	36.798	7.050	5.450	1.00	14.61
	848	NE	ARG A	106	37.271	8.435	4.915 4.831	1.00 1.00	5.55
15	849	CZ	ARG A	106	38.344	8.828	4.148	1.00	20.40
	850	NH1	ARG A	106	39.064	7.946	3.479	1.00	31.42
	851	NH2	ARG A	106	38.700	10.107	4.129	1.00	46.98 48.19
	852	Ç	ARG A	106	32.770	5.674	4.756	1.00	33.55
20	853	0	ARG A	106	32.812	5.073	3.681	1.00	52.61
20	854 855	N	CYS A	107	32.077	6.789	4.929	1.00	27.72
	856	CA	CYS A	107	31.320	7.373	3.829	1.00	41.84
	857	C	CYS A	107	32.088	8.567	3.283	1.00	22.10
	858	CB	CYS A CYS A	107	31.791	9.699	3.617	1.00	21.70
25	859	SG	CYS A CYS A	107 107	29.941	7.816	4.309	1.00	53.08
	860	Ň	HIS A	108	28.736	8.075	2.959	1.00	81.46
	861	ĊA	HIS A	108	33.097 33.951	8.301 9.338	2.461	1.00	28.20
	862	CB	HIS A	108	35.203	8.680	1.869	1.00	34.09
	863	CG	HIS A	108	36.204	9.643	1.301	1.00	40.04
30	864	CD2	HIS A	108	36.947	9.629	0.762 -0.371	1.00	35.83
	865	ND1	HIS A	108	36.593	10.766	1.460	1.00 1.00	36.86
	866	CE1	HIS A	108	37.536	11.397	0.779	1.00	36.99
	867	NE2	HIS A	108	37.767	10.725	-0.334	1.00	45.07 23.01
25	868	Ç	HIS A	108	33.251	10.165	0.774	1.00	42.71
35	869	0	HIS A	108	32.719	9.638	-0.199	1.00	37.25
	870	N	GLY A	109	33.269	11.480	0.946	1.00	49.87
	871 872	CA	GLY A	109	32.623	12.365	-0.006	1.00	29.45
	872 873	C O	GLY A	109	33.537	12.894	-1.088	1.00	26.33
40	874	Ň	GLY A TRP A	109	34.721	13.111	-0.879	1.00	19.36
	875	CA	TRP A	110 110	32.939	13.111	-2.263	1.00	35.74
	876	CB	TRP A	110	33.697 32.731	13.598	-3.404	1.00	32.65
	877	ČĞ	TRP A	110	33.447	13.903 14.390	-4.564	1.00	20.29
	878	CD2	TRP A	110	34.199	13.610	-5.792	1.00	22.58
45	879	CE2	TRP A	110	34.759	14.506	-6.731 -7.667	1.00	26.60
	880	CE3	TRP A	110	34.452	12.242	-6.864	1.00 1.00	16.42
	881	CD1	TRP A	110	33.584	15.673	-6.187	1.00	20.97
	882	NE1	TRP A	110	34.350	15.760	·7.312	1.00	16.06 29.92
50	883	CZ2	TRP A	110	35.572	14.088	-8.734	1.00	11.79
30	884	CZ3	TRP A	110	ى5 .260	11.817	-7.931	1.00	46.44
	885 886	CH2	TRP A	110	35.812	12.748	-8.853	1.00	19.66
	887	C	TRP A	110	34.565	14.791	-3.047	1.00	29.32
	888	Ň	TRP A	110	34.162	15.708	-2.335	1.00	21.14
55	889	CA	ARG A ARG A	111	35.814	14.736	-3.559	1.00	32.25
	890	CB	ARG A	111 111	36.819	15.806	-3.372	1.00	51.05
	891	ČĠ	ARG A	111	36. 294 36. 33 5	17.122	-3.911	1.00	55.38
	892	CD	ARG A	111	37.728	17.249 16.914	-5.405	1.00	82.45
	893	NE	ARG A	111	37.701	16.807	-5.919 -7.077	1.00	117.48
60	894	cz	ARG A	111	38.779	16.716	-7.377 -8.149	1.00	137.24
	895	NH1	ARG A	111	39.988	16.721	-7.601	1.00 1.00	143.04
	896	NH2	ARG A	111	38.650	16.625	-9.468	1.00	142.25
	897	,c	ARG A	111	37.110	16.070	-1.919	1.00	146.91 61.58
4 5	898	0	ARG A	111	37.239	17.225	-1.504	1.00	77.35
65	899	N	ASN A	112	37.217	15.017	-1.101	1.00	59.89
	900	CA	ASN A	112	37.433	15.116	0.363	1.00	47.67
	901	CB	ASN A	112	38.892	15.480	0.648	1.00	68.19
	902 903	CG CD1	ASN A	112	39.700	14.277	1.106	1.00	77.01
70	904	OD1 ND2	ASN A	112	39.474	13.725	2.188	1.00	77.39
, ,		1104	ASN A	112	40.669	13.866	0.282	1.00	78.90

	905	C	ASN A	112	36.433	16.068	0.984	1.00	28.46
	906	0	ASN A	112	36.705	16.745	1.990	1.00	47.00
	907 908	N · CA	TRP A	113	35.263	16.090	0.367	1.00	35.39
5	909	CB	TRP A	113 113	34.201 33.208	16.977 17.136	0.819	1.00	51.08
	910	CG	TRP A	113	32.539	18.373	-0.253 0.147	1.00 1.00	64.97
	911	CD2	TRP A	113	32.917	19.678	-0.301	1.00	81.55
	912	CE2	TRP A	113	32.014	20.570	0.303	1.00	74.85 85.26
10	913 914	CE3 CD1	TRP A TRP A	113	33.902	20.163	'-1.1 7 7	1.00	61.05
	915	NE1	TRP A	113 113	31.496 31.158	18.519	0.997	1.00	83.43
	916	CZ2	TRP A	113	32.073	19.856 21.949	1.104 0.055	1.00	83.67
	917	CZ3	TRP A	113	33.958	21.536	-1.420	1.00 1.00	96.42
15	918	CH2	TRP A	113	33.046	22.396	-0.803	1.00	72.53 92.25
13	919 920	CO	TRP A	113	33.482	16.590	2.066	1.00	46.75
	921	N	TRP A ASP A	113	33.409	15.393	2.379	1.00	35.50
	922	ČA	ASP A	114 114	32.921 32.243	17.551 17.1 7 3	2.792	1.00	63.72
••	923	CB	ASP A	114	32.177	18.380	4.025 4.943	1.00 1.00	64.61
20	924	CG	ASP A	114	33.506	18.737	5.602	1.00	86.45 98.41
	925	OD1	ASP A	114	34.402	17.872	5.707	1.00	84.34
	926 927	OD2 C	ASP A ASP A	114	33.641	19.918	6.023	1.00	109.32
	928	ŏ	ASP A ASP A	114 114	30.871	16.558	3.829	1.00	61.40
25	929	Ň	VAL A	115	30.070 30.569	17.044 15.4 6 3	3.039	1.00	81.69
	930	CA	VAL A	115	29.265	14.772	4.556 4.391	1.00 1.00	39.40
	931	CB	VAL A	115	29.491	13.274	4.126	1.00	37.88 10.52
	932 933	CG1	VAL A	115	28.209	12.621	3.617	1.00	5.47
30	934	CG2 C	VAL A VAL A	115	30.635	13.071	3.147	1.00	9.13
-	935	ŏ	VAL A VAL A	115 115	28.364 28.807	14.928 14.733	5.596	1.00	28.56
	936	Ň	TYR A	116	27.101	15.273	6.740 5.384	1.00 1.00	19.72
	937	CA	TYR A	116	26.192	15.428	6.517	1.00	37.21 46.14
35	938	CB	TYR A	116	25.652	16.857	6.574	1.00	61.34
33	939 940	CG CD1	TYR A	116	26.725	17.921	6.689	1.00	76.00
	941	CE1	TYR A TYR A	116 116	27.203 28.190	18.582	5.557	1.00	87.94
	942	CD2	TYR A	116	27.264	19.572 18.269	5.658 7.931	1.00	91.76
40	943	CE2	TYR A	116	28.255	19.255	8.041	1.00 1.00	84.35 88.13
40	944	CZ	TYR A	116	28.709	19.897	6.899	1.00	83.79
	945 946	ОH	TYR A	116	29.683	20.859	6.988	1.00	79.96
	947	C	TYR A TYR A	116 116	25.022 24.764	14.449	6.489	1.00	48.03
	948	Ň	LYS A	117	24.764	13.805 14.360	5.461 7.618	1.00 1.00	47.24
45	949	CA	LYS A	117	23.175	13.455	7.754	1.00	49.04 62.64
	950	CB	LYS A	117	21.940	14.043	7.066	1.00	84.33
	951 952	CG CD	LYS A Lys a	117	21.382	15.296	7.713	1.00	103.44
	953	CE	LYS A Lys a	117 117	20.779 20.018	15.016	9.087	1.00	122.93
50	954	NZ	LYS A	117	19.408	16.235 16.006	9.606 10.942	1.00	125.37
	955	Ç	LYS A	117	23.543	12.117	7.115	1.00 1.00	122.53 59.71
	956	O	LYS A	117	22.858	11.626	6.207	1.00	73.62
	957 958	N CA	VAL A	118	24.636	11.532	7.588	1.00	36.40
55	959	CB	VAL A VAL A	118 118	25.107 26.612	10.262	7.057	1.00	27.92
	960	CG1	VAL A	118	27.021	10.090 8.714	7.262 6.845	1.00	4.59
	961	CG2	VAL A	118	27.369	11.124	6.440	1.00 1.00	4.5 9 27.69
	962	C	VAL A	118	24.421	9.071	7.685	1.00	21.65
60	963 964	0 N	VAL A	118	24.371	8.943	8.897	1.00	23.38
00	965	ČA	ILE A ILE A	119 119	23.882	8.205	6.843	1.00	29.44
	966	CB	ILE A	119	23 <i>.2</i> 22 21.749	7.008 7.038	7.313	1.00	32.32
	967	CG2	ILE A	119	21.120	5.711	7.026 7.453	1.00 1.00	15.68 9.94
65	968	CG1	ILE A	119	21.116	8.205	7.779	1.00	16.41
UJ	969 970	CD1	ILE A	119	19.568	8.203	7.722	1.00	28.41
	970 971	C O	ILE A ILE A	119	23.817	5.818	6.605	1.00	41.89
	972	Ň	ILE A TYR A	119 120	24.159 23.073	5.901	5.424	1.00	51.23
~ ^	973	CA	TYR A	120	23.973 24.530	4.719 3.531	7.330 6.720	1.00	34.78
70	974	CB	TYR A	120	25.732	3.013	7.510	1.00 1.00	31.98 6.64
								1.00	0.04

	975	CG	TYR A	120	26.985	3.845	7.362	1.00	4.59
	976 977	CD1 CE1	TYR A TYR A	120 120	27.192 28.354	4.931	8.175	1.00	7.90
	978	CD2	TYR A	120	28.334 27.912	5.687 3.527	8.055	1.00	5.34
5	979	CE2	TYR A	120	29.085	4.271	6.413 6.270	1.00	8.49
	980	CZ	TYR A	120	29.304	5.353	7.090	1.00 1.00	23.20
	981	ОН	TYR A	120	30.467	6.077	6.927	1.00	24.78 41.99
	982	Ç	TYR A	120	23.454	2.476	6.672	1.00	39.78
10	983	0	TYR A	120	22.664	2.339	7.614	1.00	25.06
10	984 985	N CA	TYR A	121	23.406	1.748	5.564	1.00	40.70
	986	CA CB	TYR A TYR A	121 121	22,421	0.694	5.421	1.00	43.93
	987	CG	TYR A	121	21.497 20.739	0.982 2.288	4.248	1.00	37.43
	988	CD1	TYR A	121	21.387	3.511	4.367 4.161	1.00	49.95
15	989	CE1	TYR A	121	20.691	4.723	4.161	1.00 1.00	49.22
	990	CD2	TYR A	121	19.369	2.303	4.678	1.00	56.51 25.20
	991	CE2	TYR A	121	18.664	3.494	4.783	1.00	32.17
	992	CZ	TYR A	121	19.326	4.709	4.572	1.00	58.52
20	993	ОН	TYR A	121	18.632	5.904	4.685	1.00	47.56
20	994 995	CO	TYR A TYR A	121	23.095	-0.65 <i>u</i>	5.206	1.00	57.82
	996	Ň	LYS A	121 122	23.997 22.677	-0.778 -1.636	4.341	1.00	56.35
	997	CA	LYS A	122	23.216	-2.978	6.003 5.881	1.00	50.06
	998	СВ	LYS A	122	23.790	-3.497	7.209	1.00 1.00	54.50
25	999	CG	LYS A	122	24.742	-4.667	7.027	1.00	66.15 79.15
	1000	CD	LYS A	122	24.992	-5.443	8.315	1.00	81.56
	1001	CE	LYS A	122	23.821	-6.355	8.653	1.00	78.05
	1002	NZ	LYS A	122	24.119	-7.213	9.829	1.00	89.70
30	1003 1004	C	LYS A	122	22.040	-3.841	5.463	1.00	56.73
30	1004	0 N	LYS A ASP A	122	21.202	-4.210	6.289	1.00	47.59
	1006	CA	ASP A	123 123	21.978 20.911	-4.138 -4.951	4.168	1.00	66.50
	1007	CB	ASP A	123	20.768	-6.270	3.599 4.365	1.00	73.31
	1008	CG	ASP A	123	21.977	-7.186	4.190	1.00 1.00	80.64 94.21
35	1009	OD1	ASP A	123	22.334	-7.499	3.031	1.00	103.57
	1010	QD2	ASP A	123	22.568	-7.600	5.214	1.00	97.62
	1011	Ç	ASP A	123	19.591	-4.203	3.608	1.00	74.17
	1012 1013	0	ASP A	123	18.616	-4.644	4.220	1.00	66.73
40	1013	N CA	GLY A GLY A	124 124	19.571	-3.062	2.928	1.00	75.26
	1015	c c	GLY A	124	18.362 17.954	-2.265 -1.637	2.851	1.00	79.44
	1016	ŏ	GLY A	124	17.323	-0.580	4.166 4.186	1.00 1.00	80.57
	1017	N	GLU A	125	18.301	-2.295	5.268	1.00	91.15 74.63
	1018	CA	GLU A	125	17.981	-1.786	6.594	1.00	61.74
45	1019	CB	GLU A	125	18.066	-2.914	7.616	1.00	79.17
	1020	CG	GLU A	125	17.092	-4.054	7.365	1.00	98.38
	1021 1022	CD	GLU A	125	15.642	-3.619	7.478	1.00	106.78
	1023	OE1 OE2	GLU A GLU A	125	15.235	-3.167	8.570	1.00	118.36
50	1024	C	GLU A	125 125	14.907	-3.728 -0.660	6.475	1.00	110.58
	1025	ŏ	GLU A	125	18.947 20.161	-0.697	6.981 6.664	1.00	58.10
	1026	Ň	ALA A	126	18.399	0.343	7.662	1.00 1.00	30.38 50.55
	1027	CA	ALA A	126	19.185	1.490	8.088	1.00	50.55 52.07
~~	1028	СВ	ALA A	126	18.322	2.732	8.098	1.00	53.61
55	1029	C	ALA A	126	19.795	1.272	9.461	1.00	45.73
	1030	0	ALA A	126	19.077	1.194	10.459	1.00	48.02
	1031 1032	N CA	LEU A	127	21.122	1.179	9.491	1.00	34.72
	1033	CB	LEU A LEU A	127 127	21.895	0.979	10.720	1.00	30.29
60	1034	CG	LEU A	127	23.358 23.473	0.751 -0.487	10.350	1.00	15.93
	1035	CD1	LEU A	127	24.904	-0.710	9.465 9.010	1.00 1.00	4.91
	1036	CD2	LEU A	127	22.935	-1.692	10.260	1.00	4.59 16.61
	1037	С	LEU A	127	21.782	2.175	11.660	1.00	21.97
6 E	1038	0	LEU A	127	22.724	2.962	11.801	1.00	23.95
65	1039	N.	LYS A	128	20.635	2.305	12.315	1.00	19.75
	1040	CA	LYS A	128	20.391	3.427	13.205	1.00	29.37
	1041 1042	CB CG	LYS A	128	19.091	3.206	13.951	1.00	16.78
	1042	CD	LYS A LYS A	128 128	17.911	2.993	13.019	1.00	47.56
70	1044	CE	LYS A	128	16.603 15.492	2.817 2.380	13.777	1.00	56.74
			-		10.702	2.000	12.824	1.00	58 .6 8

	1045	NZ	LYS A	128	14.183	2.220	13.519	1.00	6E 70
	1046	C	LYS A	128	21.529	3.647	14.187	1.00	55.73 40.15
	1047	0	LYS A	128	22.289	4.599	14.064	1.00	53.09
5	1048	N	TYR A	129	21.647	2.757	15.159	1.00	36.41
3	1049 1050	CA CB	TYR A TYR A	129	22.707	2.860	16.144	1.00	37.61
	1051	ČG	TYR A	129 129	23.134 22.011	1.465 0.668	16.629 17.256	1.00	55.67
	1052	CD1	TYR A	129	21.225	-0.184	16.491	1.00 1.00	69.76
	1053	CE1	TYR A	129	20.152	-0.868	17.051	1.00	84.41 80.71
10	1054	CD2	TYR A	129	21.699	0.813	18.604	1.00	78.34
	1055	CE2	TYR A	129	20.632	0.136	19.172	1.00	85.65
	1056 1057	CZ	TYR A	129	19.860	-0.702	18.391	1.00	81.90
	1057	C C	TYR A TYR A	129 129	18.794	-1.369	18.952	1.00	78.93
15	1059	ŏ	TYR A	129	23.938 24.414	3. 63 5 4.513	15.664	1.00	41.39
	1060	N	TRP A	130	24.451	3.321	16.379 14.475	1.00 1.00	73.88 21.26
	1061	CA	TRP A	130	25.630	4.021	13.983	1.00	55.41
	1062	CB	TRP A	130	26.227	3.270	12.798	1.00	66.63
20	1063	CG	TRP A	130	26.560	1.867	13.090	1.00	78.03
20	1064 1065	CD2 CE2	TRP A TRP A	130	27.747	1.387	13.717	1.00	80.17
	1066	CE3	TRP A	130 130	27.652 28.889	-0.021 2.009	13.762	1.00	96.27
	1067	CD1	TRP A	130	25.807	0.770	14.244 12.791	1.00 1.00	63.46
	1068	NE1	TRP A	130	26.456	-0.371	13.189	1.00	95.81 93.15
25	1069	CZ2	TRP A	130	28.657	-0.822	14.314	1.00	106.12
	1070	CZ3	TRP A	130	29.888	1.215	14.792	1.00	70.51
	1071 1072	CH2 C	TRP A	130	29.764	-0.188	14.823	1.00	97.78
	1073	ŏ	TRP A	130 130	25.397 26.292	5.477 6.113	13.569	1.00	69.95
30	1074	Ň	TYR A	131	24.215	6.013	13.027 13.841	1.00 1.00	86.40 75.40
	1075	CA	TYR A	131	23.916	7.387	13.449	1.00	75.40 97.14
	1076	CB	TYR A	131	22.479	7.739	13.825	1.00	111.94
	1077	CG	TYR A	131	21.976	8.995	13.151	1.00	148.46
35	1078 1079	CD1 CE1	TYR A TYR A	131	21.452	8.958	11.863	1.00	154.63
55	1080	CD2	TYR A	131 131	20.988 22.025	10.111 10.223	11.242 13.800	1.00	166.01
	1081	CE2	TYR A	131	21.566	11.383	13.187	1.00 1.00	162.09 169.95
	1082	CZ	TYR A	131	21.046	11.320	11.909	1.00	172.27
40	1083	ŎН	TYR A	131	20.578	12.465	11.306	1.00	171.20
40	1084 1085	C	TYR A	131	24.854	8.424	14.048	1.00	107.44
	1086	0 N	TYR A GLU A	131 132	25.432 24.991	9.238	13.326	1.00	112.84
	1087	CA	GLU A	132	24.891 25.857	8.410 9.362	15.368 16.047	1.00 1.00	111.22
	1088	СВ	GLU A	132	26.071	8.954	17.505	1.00	114.10 121.12
45	1089	CG	GLU A	132	24.802	8.888	18.342	1.00	146.81
	1090	CD	GLU A	132	25.067	8.459	19.774	1.00	1567
	1091 1092	OE1 OE2	GLU A GLU A	132	26.243	8.195	20.104	1.00	168.06
	1093	C	GLU A	132 132	24.100 27.212	8.386 9.442	20.565 15.359	1.00	164.60
50	1094	ŏ	GLU A	132	27.715	10.523	15.090	1.00 1.00	112.41 126.08
	1095	N	ASN A	. 133	27.792	8.286	15.065	1.00	107.15
•	1096	CA	ASN A	133	29.101	8.246	14.436	1.00	110.99
	1097	CB	ASN A	133	29.828	6.972	14.874	1.00	132.56
5 5	1098 16: 1 9	CG OD1	asn a Asn a	133 133	29.903 30.195	6.843	16.381	1.00	152.00
-	1100	ND2	ASN A	133	29.636	7.810 5.653	17.084 16.882	1.00	156.21
	1101	C	ASN A	133	29.071	8.366	12.913	1.00 1.00	104.20 103.70
	1102	0	ASN A	133	28.344	7.653	12.236	1.00	103.53
60	1103	N	HIS A	134	29.885	9.274	12.388	1.00	108.74
00	1104 1105	CA	HIS A	134	29.987	9.520	10.954	1.00	130.31
	1106	CB CG	HIS A HIS A	134 134	30.880 30.457	10.729	10.703	1.00	148.82
	1107	CD2	HIS A	134	31.030	11.949 12.601	11.454	1.00	166.98
	1108	ND1	HIS A	134	29.283	12.620	12.493 11.183	1.00 1.00	171 <i>,2</i> 9 179,56
65	1109	CE1	HIS A	134	29.153	13.629	12.026	1.00	185.16
	1110	NE2	HIS A	134	30.196	13.641	12.829	1.00	183.14
	1111	C	HIS A	134	30.572	8.320	10.242	1.00	130.17
	1112 1113	O N	HIS A ASN A	134	30.194	8.013	9.120	1.00	144.97
70	1114	CA	ASN A	135 135	31.506 32.133	7.668 6.470	10.891 10.351	1.00	115.50
-	• •		7.0,1		· 100	0.770	10.331	1.00	106.66

	1115 1116	CB CG	ASN A	135 135	33.641 34.357	6.677 6.732	10.201 11.535	1.00 1.00	111.41
	1117	OD1	ASN A	135	33.734	6.607	12,590	1.00	121.66 137.22
_	1.118	ND2	ASN A	135	35.671	6.919	11.493	1.00	131.58
5	1119	C	ASN A	135	31.848	5.256	11.226	1.00	98.67
	1120 1121	0 N	ASN A	135 136	31.560 31.914	5.429 4.084	12.414 10.657	1.00	95.00
	1122	ČA.	ILE A	136	31.590	2.901	11.441	1.00 1.00	84.56 68.70
	1123	CB	ILE A	136	30.615	2.005	10.689	1.00	70.57
10	1124	CG2	ILE A	136	30.242	0.824	11.556	1.00	57.24
	1125 1126	CG1 CD1	ILE A	136 136	29.371 28.315	2.809 1.994	10.308 9.607	1.00	76.41
	1127	Č.	ILE A	136	32.825	2.108	11.771	1.00 1.00	81.35 67.79
	1128	0	ILE A	136	33.484	1.575	10.879	1.00	75.89
15	1129	N	SER A	137	33.153	2.051	13.057	1.00	64.01
	1130 1131	CA CB	SER A	137 137	34.327 35.240	1.314 2.228	13.512	1.00	50.08
	1132	OG	SER A	137	36.435	1.547	14.319 14.654	1.00 1.00	42.18 74.65
••	1133	C	SER A	137	33.882	0.137	14.366	1.00	40.13
20	1134	0	SER A	137	33.257	0.331	15.402	1.00	31.91
	1135 1136	N CA	ILE A	138 138	34.172 33.767	-1.079 -2.272	13.915	1.00	47.57
	1137	CB	ILE A	138	32.849	-2.272 -3.173	14.646 13.801	1.00 1.00	55.59 45.34
	1138	CG2	ILE A	138	32.360	-4.317	14.646	1.00	52.83
25	1139	CG1	ILE A	138	31.640	-2.378	13.310	1.00	55.63
	1140 1141	CD1 C	ILE A	138 138	30.680 35.014	-3.166 -3.039	12.457	1.00	59.56
	1142	ŏ	ILE A	138	35.542	-3.824	15.023 14.243	1.00 1.00	69.36 86.80
••	1143	N	THR A	139	35.481	-2.793	16.238	1.00	80.29
30	1144	CA	THR A	139	36.687	-3.412	16.765	1.00	71.05
	1145 1146	CB OG1	THR A	139 139	36.824 35.584	-3.094	18.243	1.00	65.21
	1147	CG2	THR A	139	37.152	-3.396 -1.610	18.894 18.429	1.00 1.00	63.19 37.67
	1148	С	THR A	139	36.727	-4.906	16.577	1.00	73.17
35	1149	0	THR A	139	37.633	-5.439	15.927	1.00	72.09
	1150 1151	N CA	ASN A	140 140	35.731 35.689	-5.585 -7.021	17.126	1.00	71.99
	1152	CB	ASN A	140	35.704	-7.615	17.012 18.427	1.00 1.00	74.50 83.94
40	1153	CG	ASN A	140	37.023	-8.292	18.747	1.00	102.78
40	1154	OD1	ASN A	140	37.329	-9.296	18.114	1.00	129.44
	1155 1156	ND2 C	ASN A	140 140	37.842 34.509	-7. 797 -7.489	19.666	1.00	102.21
	1157	ŏ	ASN A	140	33.351	-7.49 5 -7.495	16.134 16.568	1.00 1.00	66.79 67.94
	1158	N	ALA A	141	34.834	-7.874	14.888	1.00	51.28
45	1159	CA	ALA A	141	33.851	-8.305	13.887	1.00	50.10
	1160 1161	CB C	ALA A	141 141	34.536 33.037	-8.441 -9.568	12.546	1.00	44.66
	1162	ŏ	ALA A	1/11	22 205	-10.379	14.167 15.013	1.00 1.00	57.39 76.44
70	1163	N	THR A	142 -	~ 31.940	-9.721	13.424	1.00	63.44
50	1164	CA	THR A	142	31.029	-10.864	13.548	1.00	68.80
	1165 1166	CB OG1	THR A	142 142	29.830 30.292	-10.522 -9.914	14.429	1.00	56.28
	1167	CG2	THR A	142	29.038	-9.914 -11.771	15. 63 7 14.756	1.00 1.00	69.20 63.69
	1168	С	THR A	142	30.476	-11.284	12.186	1.00	77.84
55	1169	0	THR A	142	30.350	-10.467	11.275	1.00	84.69
	1170 1171	N CA	VAL A	143 143	30.133 29.594	-12.562 -13.071	12.053	1.00	80.43
	1172	CB	VAL A	143	29.347	-13.071 -14.600	10.800 10.870	1.00 1.00	75.62 62.57
60	1173	CG1	VAL A	143	28.297	-14.907	11.934	1.00	69.07
60	1174	CG2	VAL A	143	28.903	-15.123	9.516	1.00	78.52
	1175 1176	C	VAL A	143 143	28.282	-12.361	10.472	1.00	73.71
	1177	Ň	GLU A	144	27.893 27.593	-12.285 -11.846	9.307 11.491	1.00 1.00	85.08 65.50
C	1178	CA	GLU A	144	26.347	-11.130	11.245	1.00	78.86
65	1179	CB	GLU A	144	25.554	-10.974	12.544	1.00	88.26
	1180 1181	CG CD	GLU A	144	24.140 23.389	-10.450 -10.200	12.348	1.00	123.20
	1182	OE1	GLU A	144 144	23.369	-10. 299 -10.598	13.656 14.717	1.00 1.00	142.61 141.13
70	1183	OE2	GLU A	144	22.212	-9.883	13.620	1.00	155.89
70	1184	С	GLU A	144	26.611	-9.767	10.616	1.00	84.50

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	1185	0	GLU A	144	25.793	-9 .241	9.855	1.00	86.40
	1186	N	ASP A	145	27.764	-9.198	10.943	1.00	83.52
	1187	CA	ASP A	145	28.139	-7.913	10.383	1.00	73.54
_	1188	CB	ASP A	145	29.429	-7.402	11.033	1.00	81.77
5	1189	CG	ASP A	145	29.191	-6.826	12.430	1.00	98.36
	1190	OD1	ASP A	145	28.336	-5.914	12.559	1.00	102.22
	1191	OD2	ASP A	145	29.856	-7.280	13.394	1.00	95.71
	1192	С	ASP A	145	28.317	-8.028	8.875	1.00	
	1193	0	ASP A	145	28.626	-7.053	8.211	1.00	65.16
10	1194	N	SER A	146	28.112	-9.224	8.337		74.60
	1195	CA	SER A	146	28.246	-9.460	6.906	1.00	63.10
	1196	CB	SER A	146	28.403	-10.959		1.00	51.02
	1197	OG	SER A	146	29.671		6.619	1.00	62.55
	1198	č	SER A			-11.452	7.030	1.00	53.04
15	1199	ŏ	SER A	146	26.997	-8.949	6.221	1.00	50.62
13	1200	N	OLY A	146	25.935	-8.865	6.848	1.00	44.95
	1200		GLY A	147	27.130	-8.609	4.942	1.00	48.93
		CA	GLY A	147	25.992	-8.119	4.185	1.00	55.32
	1202	C	GLY A	147	26.389	-7.039	3.199	1.00	60.64
20	1203	0	GLY A	147	27.587	-6.725	3.051	1.00	55.89
20	1204	N	THR A	148	25.396	-6.477	2.510	1.00	61.14
	1205	CA	THR A	148	25.665	-5.415	1.540	1.00	66.29
	1206	CB	THR A	148	24.735	-5.502	0.318	1.00	67.47
	1207	OG1	THR A	148	23.514	-4.813	0.604	1.00	89.27
0.5	1208	CG2	THR A	148	24.414	-6.954	-0.006	1.00	53.85
25	1209	С	THR A	148	25.442	-4.064	2.229	1.00	60.43
	1210	0	THR A	148	24.373	-3.805	2.793	1.00	48.98
	1211	N	TYR A	149	26.461	-3.214	2.203	1.00	56.49
	1212	CA	TYR A	149	26.371	-1.911	2.836	1.00	
	1213	CB	TYR A	149	27.600	-1.648	3.726		46.76
30	1214	CG	TYR A	149	27.679	-2.436	5.010	1.00	50.51
	1215	CD1	TYR A	149	28.197	-3.727		1.00	37.62
	1216	CE1	TYR A	149	28.288	-4.446	5.030	1.00	38.64
	1217	CD2	TYR A	149	27. <u>2</u> 52		6.214	1.00	21.54
	1218	CE2	TYR A	149	27.232 27.336	-1.882	6.211	1.00	27.02
35	1219	CZ	TYR A			-2.589	7.393	1.00	25.84
23	1220	OH	TYR A	149	27.854	-3.868	7.390	1.00	22.38
	1221	C		149	27.923	-4.562	8.573	1.00	47.89
	1222	ŏ	TYR A	149	26.329	-0.824	1.775	1.00	47.29
	1223	Ñ	TYR A	149	26.626	-1.059	0.590	1.00	37.99
40	1224		TYR A	150	25.962	0.369	2.225	1.00	35.54
40		CA	TYR A	150	25.947	1.547	1.380	1.00	37.17
	1225	CB	TYR A	150	25.029	1.341	0.165	1.00	20.88
	1226	CG	TYR A	150	23.546	1.438	0.440	1.00	11.30
	1227	CD1	TYR A	150	22.897	2.667	0.465	1.00	12.45
45	1228	CE1	TYR A	150	21.518	2.751	0.712	1.00	32.37
45	1229	CD2	TYR A	150	22.789	0.299	0.668	1.00	24.35
	1230	CE2	TYR A	150	21.412	0.374	0.909	1.00	20.64
	1231	CZ	TYR A	150	20.784	1.599	0.933	1.00	30.87
	1232	ОН	TYR A	150	19.428	1.673	1.174	1.00	44.40
	1233	С	TYR A	150	25.492	2.711	2.250	1.00	39.54
50	1234	0	TYR A	150	24.661	2.544	3.170	1.00	10.94
	1235	N	CYS A	151	26.062	3.882	1.987	1.00	36.69
	1236	CA	CYS A	151	25.705	5.052	2.757	1.00	45.12
	1237	С	CYS A	151	25.007	6.072	1.908		
	1238	0	CYS A	151	25.146	6.112	0.686	1.00	51.21
55	1239	CB	CYS A	151	26.931	5.677		1.00	60.75
	1240	SG	CYS A	151	28.208	6.239	3.410	1.00	44.14
	1241	N	THR A	152	24.258	6.891	2.230	1.00	79.82
	1242	CA	THR A	152	23.500		2.606	1.00	48.42
	1243	CB	THR A			7.959	1.949	1.00	39.06
60	1244	001	THR A	152	22.068	7.517	1.650	1.00	43.65
•	1245	CG2	THR A	152	21.399	8.531	0.891	1.00	41.96
	1246			152	21.310	7.257	2.842	1.00	52.65
	1247	C	THR A	152	23.555	9.204	2.825	1.00	38.12
		0	THR A	152	23.025	9.224	3.943	1.00	25.44
65	1248	N	GLY A	153	24.215	10.236	2.307	1.00	56.51
G.J	1249	CA	GLY A	153	24.377	11.477	3.048	1.00	57.72
	1250	Ç	GLY A	153	24.335	12.680	2.112	1.00	54.16
	1251	0	GLY A	153	24.362	12.540	0.903	1.00	50.60
	1252	N _.	LYS A	154	24.309	13.842	2.706	1.00	38.84
70	1253	CA	LYS A	154	24.227	14.969	1.840	1.00	51.33
70	1254	CB	LYS A	154	23.115	15.878	2.356	1.00	63.30
									J

	1255 1256	CG	LYS		23.445	17.360	2.388	1.00	72.63
	1250	CE ·	LYS A		22.595 23.004	18.054	3.439	1.00	102.12
	1258	NZ NZ	LYS		22.404	19.508 20.128	3.589 4.797	1.00	114.39
5	1259	Ċ	LYS		25.591	15.650	1.647	1.00 1.00	116.75
	1260	Ö	LYS /		26.393	15.769	2.565	1.00	43.23 25.84
	1261	N	VAL A	A 155	25.799	16.110	0.410	1.00	50.07
	1262	CA	VAL. A		27.053	16.754	0.017	1.00	48.54
10	1263	СВ	VAL /		27.920	15.801	-0.810	1.00	44.27
10	1264	CG1	VAL /		29.142	16.517	-1.363	1.00	33.53
	1265 1266	CG2 C	VAL A		28.341 26.752	14.619	0.032	1.00	57.29
	1267	ŏ	VAL A		26.732 26.127	18.008 17.926	-0.791 -1.839	1.00 1.00	67.17
	1268	Ň	TRP A		27.200	19.158	-0.290	1.00	75.50 71.27
15	1269	CA	TRP /		26.950	20.433	-0.941	1.00	74.25
	1270	CB	TRP A		27.792	20.531	-2.227	1.00	82.77
	1271	CG	TRP /		27.663	21.880	-2.856	1.00	95.08
	1272	CD2	TRP /		27.991	23.118	-2.237	1.00	99.06
20	1273 1274	CE2 CE3	TRP /		27.707	24.146	-3.172	1.00	109.06
20	1275	CD1	TRP A		28.499 27.202	23.466 22.187	-0.981 -4.115	1.00	92.83
	1276	NE1	TRP A		27.226	23.548	-4.308	1.00 1.00	103.95
	1277	CZ2	TRP A		27.915	25.505	-2.883	1.00	101.14 117.16
~~	1278	CZ3	TRP A	A 156	28.708	24.820	-0.691	1.00	111.82
25	1279	CH2	TRP A		28.415	25.823	-1.644	1.00	117.54
	1280	C	TRP A		25.451	20.622	-1.252	1.00	77.62
	1281 1282	0 N	TRP A		25.074	20.840	-2.391	1.00	86.35
	1283	CA	GLN A		24.612 23.148	20.526 20.731	-0.216 -0.292	1.00	65.28
30	1284	CB	GLN A		22.904	22,189	-0.292 -0.665	1.00 1.00	81.65 97.92
	1285	CG	GLN A		23.502	23.199	0.312	1.00	117.66
	1286	CD	GLN A	157	23.208	24.631	-0.086	1.00	136.93
	1287	OE1	GLN A		22.533	24.882	-1.084	1.00	146.04
35	1288	NE2	GLN A		23.616	25.725	0.549	1.00	141.98
33	1289 1290	C	GLN A		22.274	19.790	-1.165	1.00	79.89
	1291	Ň	LEU A		21.156 22.779	20.148 18.632	-1.533 -1.485	1.00	84.84
	1292	ĊA	LEU A	158	22.000	17.633	-1.465 -2.253	1.00 1.00	73.68 79.20
	1293	СВ	LEU A	158	22.364	17.659	-3.749	1.00	79.50
40	1294	CG	LEU A	158	22.096	18.967	-4.507	1.00	86.09
	1295	CD1	LEU A		22.474	18.815	-5.972	1.00	76.62
	1296 1297	CD2 C	LEU A	158	20.647	19.379	-4.373	1.00	92.41
	1298	ŏ	LEU A		22.262 23.390	16.262 15.914	-1.673	1.00	70.21
45	1299	Ň	ASP A		21.236	15.470	-1.325 -1.538	1.00 1.00	65.09 60.67
	1300	CA	ASP A		21.404	14.148	-0.999	1.00	55.55
	1301	CB	ASP A	159	20.088	13.617	-0.446	1.00	67.04
	1302	CG	ASP A	159	19.493	14.534	0.596	1.00	100.18
50	1303	OD1	ASP A		20.141	14.767	1.640	1.00	107.25
30	1304 1305	OD2 C	ASP A		18.375	15.034	0.368	1.00	120.77
	1306	ŏ	ASP A		21.937 21.662	13.199 13.379	-2.057 -3.258	1.00	59.79
	1307	Ň	TYR A		22.692	12.198	-0.256 -1.619	1.00 1.00	71.48
	1308	CA	TYR A		23.237	11.218	-2.545	1.00	46.99 36.10
55	1309	CB	TYR A		24.620	11.639	-3.026	1.00	27.20
	1310	CG	TYR A		24.661	13.032	-3.599	1.00	48.59
	1311 1312	CD1 CE1	TYR A		24.780	14.143	-2.770	1.00	67.84
	1313	CD2	TYR A		24.805 24.570	15.440	-3.297	1.00	85.53
60	1314	CE2	TYR A		24.570	13.246 14.538	-4.970 -5.507	1.00	46.32
	1315	CZ	TYR A		24.713	15.630	-4.665	1.00 1.00	59.84 78.07
	1316	OH	TYR A	160	24.740	16.912	-5.178	1.00	80.23
	1317	C	TYR A	160	23.314	9.852	-1.881	1.00	41.50
65	1318	0	TYR A		23.085	9.729	-0.675	1.00	33.36
ÛĴ	1319 1320	N CA	GLU A		23.623	8.830	-2.675	1.00	46.21
	1321	CB	GLU A		23.725	7.469 6.733	-2.173	1.00	42.10
	1322	CG	GLU A		22.425 22.451	6.733 5.247	-2.462 -2.195	1.00	40.63
	1323	CD	GLU A		21.042	4.640	-2.195 -2.132	1.00 1.00	72.70 87.13
70	1324	OE1	GLU A		20.932	3.391	-2.193	1.00	96.87

	1325	OE2	GLU A	161	20.049	5.405	-2.006	1.00	69.68
	1326	C	GLU A	161	24.898	6.793	-2.864	1.00	48.06
	1327	O .	GLU A	161	25.040	6.878	-4.080	1.00	53.65
_	1328	N	SER A	162	25.750	6.146	-2.079	1.00	55.15
5	1329	CA	SER A	162	26.933	5.475	-2.612	1.00	57.03
	1330	CB	SER A	162	27.968	5.246	-1.498	1.00	68.17
	1331	og.	SER A	162	27.499	4.339	-0.501	1.00	46.93
	1332	C	SER A	162	26.572	4.138	-3.230	1.00	58.42
10	1333	0	SER A	162	25.476	3.615	-3.020	1.00	48.37
IU	1334	N	GLU A	163	27.498	3.587	-4.002	1.00	65.57
	1335 1336	CA CB	GLU A	163	27.268	2.290	-4.619	1.00	70.23
	1337	CG	GLU A	163	28.356	1.990	-5.650	1.00	87. 7 7
	1337 1338	CD	GLU A GLU A	163	28.293	2.834	-6.909	1.00	103.75
15	1339	OE1	GLU A	163 163	27.121 27.060	2.453 1.281	-7.797	1.00	115.27
	1340	OE2	GLU A	163	26.262	3.323	-8.229	1.00	111.84
	1341	C	GLU A	163	27.366	1.282	-8.062 -3.491	1.00	129.74
	1342	ŏ	GLU A	163	28.244	1.387	-3.491	1.00 1.00	70.72
	1343	Ň	PRO A	164	26.460	0.300	-3.448	1.00	89.57
20	1344	CD	PRO A	164	25.401	-0	-4.397	1.00	55.48 62.15
	1345	CA	PRO A	164	26.538	-0.684	-2.369	1.00	41.51
	1346	CB	PRO A	164	25.363	-1.606	-2.663	1.00	42.71
	1347	CG	PRO A	164	25.250	-1.532	-4.128	1.00	64.09
	1348	С	PRO A	164	27.877	-1.409	-2.399	1.00	38.62
25	1349	0	PRO A	164	28.585	-1.386	-3.426	1.00	31.41
	1350	N	LEU A	165	28.234	-2.022	-1.268	1.00	33.57
	1351	CA	LEU A	165	29.498	-2.753	-1.151	1.00	25.38
	1352	СВ	LEU A	165	30.540	-1.879	-0.490	1.00	26.45
30	1353	CG	LEU A	165	31.924	-2.483	-0.322	1.00	25.16
30	1354	CD1	LEU A	165	32.619	-2.579	-1.655	1.00	29.84
	1355 1356	CD2	LEU A LEU A	165	32.736	-1.587	0.602	1.00	42.13
	1357	C	LEU A LEU A	165	29.278	-3.983	-0.306	1.00	26.10
	1358	Ň	ASN A	165 166	28.794 29.618	-3.876 -5.152	0.815	1.00	33.23
35	1359	CA	ASN A	166	29.400	-5.152 -6.398	-0.838 -0.106	1.00	40.53
	1360	CB	ASN A	166	29.257	-7.59 5	-1.049	1.00 1.00	50.87
	1361	CG	ASN A	166	27.875	-7.698	-1.649	1.00	69.69 86.10
	1362	OD1	ASN A	166	26.895	-7.260	-1.034	1.00	58.55
	1363	ND2	ASN A	166	27.799	-8.292	-2.839	1.00	110.79
40	1364	C	ASN A	166	30.537	-6.664	0.833	1.00	48.09
	1365	0	ASN A	166	31.703	-6.667	0.416	1.00	40.29
	1366	N _.	ILE A	167	30.193	-6.908	2.094	1.00	46.84
	1367	CA	ILE A	167	31.191	-7.165	3.119	1.00	53.30
45	1368	CB	ILE A	167	31.192	-6.039	4.156	1.00	54.88
43	1369	CG2	ILE A	167	31.949	-6.458	5.383	1.00	47.53
	1370 1371	CG1 CD1	ILE A	167	31.816	-4.791	3.545	1.00	48.70
	1372	C	ILE A	167	31.781	-3.603	4.447	1.00	54.75
	1373	ŏ	ILE A	167 167	30.945 29.862	-8.492 8.734	3.815	1.00	59.98
50	1374	Ň	THR A	168	29.002 31.957	-8.731 -9.353	4.388	1.00	39.94
	1375	ČA	THR A	168	31.835	-10.666	3.777 4.386	1.00 1.00	61.65
	1376	CB	THR A	168	32.052	-11.774	3.343	1.00	68.33
	1377	OG1	THR A	168	31.627	-11.306	2.058	1.00	80.46 92.03
	1378	CG2	THR A	168	31.239	-13.010	3.704	1.00	94.56
55	1379	C	THR A	168	32.829	-10.891	5.515	1.00	60.61
	1380	0	THR A	168	34.031	-10.870	5.346	1.00	54.25
	1381	N	VAL A	169	32.313	-11.331	6.660	1.00	57.24
	1382	CA	VAL A	169	33.143	-11.638	7.820	1.00	64.14
60	1383	CB	VAL A	169	32.567	-11.028	9.083	1.00	54.63
60	1384	CG1	VAL A	169	33.436	-11.381	10.261	1.00	75.25
	1385	CG2	VAL A	169	32.470	-9.533	8.929	1.00	61.93
	1386	C	VAL A	169	33.112	-13.156	7.950	1.00	73.51
	1387	0	VAL A	169	32.044	-13.739	8.173	1.00	77.56
65	1388 1389	N CA	ILE A	170	34.268	-13.801	7.815	1.00	75.88
55	1390	CA CB	ILE A	170	34.312	-15.259	7.873	1.00	80.16
	1391	CG2	ILE A	170	35.341	-15.815	6.866	1.00	75.70
	1392	CG1		170	34.778	-15.807	5.465	1.00	70.82
	1393	CD1	ILE A ILE A	170 170	36. 633	-15.007 -15.518	6.932	1.00	90.89
70	1394	Č.	ILE A	170	37.719 34.568	-15.518 -15.870	6.004	1.00	107.17
		_	1000		UT.JU0	-15.879	9.246	1.00	87.00

	1395	o	ILE A	17.0	35.373	-15.415	10.042	1.00	96.41
	1396	N	LYS A	171	33.843	-16.956	9.475	1.00	84.91
	1397 1398	CA CB	LYS A	171 171	34.002 32.777	-17.747 -18.646	10.684 10.912	1.00	77.44
5	1399	ČĞ	LYS A	171	32.895	-19.571	12.108	1.00 1.00	69.57
	1400	CD	LYS A	171	32.836	-18.812	13.422	1.00	99.45 104.18
	1401	CE	LYS A	171	32.865	-19.773	14.611	1.00	104.74
	1402	NZ	LYS A	171	32.737	-19.061	15.914	1.00	93.90
10	1403 1404	C	LYS A	171	35.260	-18.572	10.523	1.00	84.98
10	1405	N	ALA A	171 172	35.628 35.970	-18.860 -19.012	9.376 11.575	1.00 1.00	94.71
	1406	CA	ALA A	172	37.223	-19.690	11.278	1.00	87.21 95.69
	1407	CB	ALA A	172	38.361	-18.758	11.670	1.00	93.23
1.5	1408	C	ALA A	172	37.489	-21.071	11.877	1.00	105.19
15	1409	0	ALA A	172	37.954	-21.216	13.004	1.00	112.63
	1410 1411	N CD	PRO A	173 173	37.149	-22.090	11.058	1.00	110.62
	1412	CA	PRO A	173	35.763 37.466	-22.015 -23.510	10.625 11.384	1.00 1.00	99.89
	1413	CB	PRO A	173	36.690	-24.249	10.308	1.00	115.87 108.18
20	1414	CG	PRO A	173	35.438	-23.407	10.162	1.00	104.37
	1415	Ç	PRO A	173	38.974	-23.790	11.504	1.00	128.43
	1416	0	PRO .A	173	39.763	-23.104	10.878	1.00	141.54
	1417 1418	N CA	ARG A	174	39.371	-24.790	12.289	1.00	133.44
25	1419	CB	ARG A	174 174	40.784 41.404	-25.147 -24.373	12.416	1.00	142.76
	1420	ČĞ	ARG A	174	40.646	-24.535	13.578 14.896	1.00 1.00	151.84 162.79
	1421	CD	ARG A	174	40.099	-23.221	15.420	1.00	169.70
	1422	NE	ARG A	174	38.922	-23.410	16.282	1.00	176.81
20	1423	CZ	ARG A	174	38.907	-23.284	17.609	1.00	177.27
30	1424 1425	NH1	ARG A	174	40.007	-22.942	18.271	1.00	174.36
	1426	NH2 C	ARG A ARG A	174 174	37.770 40.973	-23.499 26.657	18.277	1.00	178.48
	1427	ŏ	ARG A	174	40.343	-26.657 -27.476	12. 6 20 11.946	1.00 1.00	148.93
	1428	Č1	NAG A	221	48.150	13.699	-5.031	1.00	150.68 63.44
35	1429	C2	NAG A	221	47.709	15.109	-4.571	1.00	53.07
	1430	N2	NAG A	221	46.282	15.294	-4.715	1.00	54.52
	1431	C7	NAG A	221	45.470	14.819	-3.771	1.00	67.27
	1432 1433	O7 C8	NAG A NAG A	221 221	45.884 43.972	14.210	-2.774	1.00	51.25
40	1434	cs	NAG A	221	43.972 48.484	15.033 16.177	-3.951 -5.342	1.00 1.00	58.18
	1435	03	NAG A	221	48.035	17.468	-4.966	1.00	64.80 76.76
	1436	C4	NAG A	221	49.919	15.918	-4.908	1.00	84.55
	1437	04	NAG A	221	50.874	16.976	-5.150	1.00	121.48
45	1438 1439	C5 O5	NAG A	221	50.354	14.610	-5.540	1.00	75.06
43	1440	C6	NAG A NAG A	221 221	49.589 51.837	13.531 14.319	-4.944 5.314	1.00	65.34
	1441	06	NAG A	221	52.240	13.109	-5.314 -5.940	1.00 1.00	72.88 79.15
	1442	C1	NAG A	222	50.797	17.958	-6.068	1.00	145.53
50	1443	C2	NAG A	222	50.822	19.497	-5.910	1.00	155.10
50	1444	N2	NAG A	222	49.525	20.056	-6.240	1.00	159.26
	1445 1446	C7	NAG A	222	48.710	20.465	-5.270	1.00	165.01
	1447	O7 C8	NAG A NAG A	222 222	48.999	20.393	-4.072 5.000	1.00	169.69
	1448	C3	NAG A	222	47.367 51.905	21.040 20.174	-5.688 -6.746	1.00	162.00
55	1449	03	NAG A	222	51.976	21.552	-6.412	1.00	158.11 158.38
	1450	C4	NAG A	222	53.236	19.510	-6.450	1.00	161.49
	1451	04	NAG A	∠22	54.266	20.119	-7.216	1.00	161.28
	1452 1453	C5	NAG A	222	53.108	18.028	-6.799	1.00	162.76
60	1454	O5 C6	NAG A NAG A	222 222	52.123	17.403	-5.946	1.00	157.35
- •	1455	06	NAG A	222	54.409 54.197	17.273 15.869	-6.600 -6.619	1.00 1.00	163.69 157.92
	1456	C1	NAG A	242	43.365	-3.262	-14.810	1.00	13.23
	1457	C2	NAG A	242	43.041	-2.260	-15.917	1.00	5.53
65	1458	N2	NAG A	242	44.141	-1.343	-16.143	1.00	9.70
65	1459	C7	NAG A	242	45.252	-1.749	-16.754	1.00	29.25
	1460 1461	O7 C8	NAG A	242	45.439	-2.917	-17.133	1.00	32.16
	1462	cs cs	NAG A NAG A	242 242	46.337 41.793	-0.695 -1.489	-16.957	1.00	12.96
	1463	O3	NAG A	242	41.435	-0.559	-15.507 -16.510	1.00 1.00	4.59 15.24
70	1464	C4	NAG A	242	40.615	-2.416	-15.249	1.00	11.27

	1465 1466 1467	O4 C5 O5	NAG A NAG A NAG A	242 242 242	39.565 41.027 42.281	-1.641 -3.581 -4.195	-14.619 -14.306	1.00	13.74 16.30
5	1468 1469 1470	C6 . O6 C1	NAG A NAG A	242 242	40.007 39.736	-4.698 -5.116	-14.704 -14.278 -12.948	1.00 1.00 1.00	7.58 28.55 38.66
	1471 1472 1473	C2 N2 C7	NAG A NAG A NAG A	243 243 243	38.610 37.449 36.919	-1.048 -0.610 -1.742	-15.431 -14.570 -13.845	1.00 1.00 1.00	38.51 39.03 47.25
10	1474 1475 1476	07 C8 C3	NAG A NAG A NAG A NAG A	243 243 243	36.991 37.502 36.416	-1.735 -0.806 -2.926	-12.517 -11.885 -11.769	1.00 1.00 1.00	62.38 63.20 77.74
15	1477 1478 1479	03 C4 O4	NAG A NAG A NAG A	243 243 243 243	36.389 35.272 37.029	0.062 0.474 1.275	-15.450 -14.669 -16.133	1.00 1.00 1.00	52.71 54.98 40.14
	1480 1481 1482	C5 O5 C6	NAG A NAG A NAG A	243 243 243 243	36.079 38.284 39.196	1.889 0.828 0.104	-17.033 -16.909 -16.046	1.00 1.00 1.00	74.71 29.29 36.06
20	1483 1484 1485	O6 C1 C2	NAG A MAN A MAN A	243 243 244 244	39.063 40.407 35.717	2.012 1.653 3.208	-17.448 -17.751 -16.771	1.00 1.00 1.00	35.70 34.26 75.57
	1486 1487 1488	O2 C3 O3	MAN A MAN A MAN A	244 244 244 244	35.709 34.884 35.181	4.009 3.345 5.431	-18.090 -19.043 -17.820	1.00 1.00 1.00	81.10 66.91 79.87
25	1489 1490 1491	C4 O4 C5	MAN A MAN A MAN A	244 244 244 244	35.162 33.782 33.238 33.918	6.216 5.322 6.611	-19.009 -17.211 -16.994	1.00 1.00 1.00	58.10 73.02 79.27
30	1492 1493 1494	O5 C6 O6	MAN A MAN A MAN A	244 244 244 244	34.401 32.626	4.560 3.215 4.463 3.523	-15.890 -16.159 -15.080	1.00 1.00 1.00	70.92 80.43 62.83
	1495 1496 1497	C1 C2 N2	NAG A NAG A NAG A	274 274 274 274	31.720 56.076 57.346 58.518	-21.009 -21.243	-15.638 -1.119 -0.277	1.00 1.00 1.00	93.61 118.55 122.52
35	1498 1499 1500	C7 O7 C8	NAG A NAG A NAG A	274 274 274 274	59.434 59.341 60.642	-20.916 -20.096 -19.596	-1.059 -0.559 0.555	1.00 1.00 1.00	104.98 87.55 87.40
	1501 1502 1503	C3 C3 C4	NAG A NAG A NAG A	274 274 274 274	57.521 58.252 56.155	-19.783 -22.673 -22.494	-1.417 0.320 1.568	1.00 1.00 1.00	88.80 134.44 158.45
40	1504 1505 1506	O4 C5 O5	NAG A NAG A NAG A	274 274 274 274	56.251 55.035 54.951	-23.387 -24.825 -22.969 -21.543	0.619 0.491 -0.345	1.00 1.00 1.00	135.00 133.45 136.04
45	1507 1508 1509	C6 O6 C1	NAG A NAG A FCA A	274 274 275	53.668 52.628 59.339	-23.483 -22.635 -23.324	-0.442 0.076 -0.387 1.916	1.00 1.00 1.00	130.02 139.67 144.24
	1510 1511 1512	C2 C3 C4	FCA A FCA A FCA A	275 275 275	59.905 60.762 61.991	-22.923 -21.695 -21.833	3.289 3.251 2.283	1.00 1.00 1.00 1.00	166.18 176.23 178.46
50	1513 1514 1515	C5 C6 O2	FCA A FCA A FCA A	275 275 275	61.389 62.389 58.772	-22.191 -22.620 -22.721	0.896 -0.196 4.211	1.00 1.00 1.00	172.76 176.96 180.24
	1516 1517 1518	O3 O4 O5	FCA A FCA A FCA A	275 275 275	61.269 62.910 60.459	-21.376 -22.849 -23.282	4.553 2.754 0.968	1.00 1.00 1.00	187.28 178.44 169.66 169.81
55	1519 1520 1521	C1 C2 N2	NAG A NAG A NAC A	276 276 276	57.235 56.691 55.572	-25.594 -27.020 27.068	1.103 1.226 2.154	1.00 1.00 1.00	98.00 98.05 97.91
60	1522 1523 1524	C7 O7 C8	NAG A NAG A NAG A	276 276 276	54.356 54.123 53.223	-27.358 -27.596 -27.391	1.694 0.498 2.716	1.00 1.00 1.00	98.05 98.12 97.73
	1525 1526 1527	C3 O3 C4	NAG A NAG A NAG A	276 276 276	57.782 57.292 59.057	-28.020 -29.346 -27.855	1.658 1.498 0.815	1.00 1.00 1.00	98.00 98.03 97.83
65	1528 1529 1530	O4 C5 O5	NAG A NAG A NAG A	276 276 276	60.118 59.467 58.367	-28.595 -26.388 -25.586	1.409 0.717 0.218	1.00 1.00 1.00	98.08 97.92 98.07
70	1531 1532 1533	C6 O6 C1	NAG A NAG A NAG A	276 276 340	60.628 60.565 39.040	-26.186 -24.929 -8.595	-0.248 -0.904 19.969	1.00 1.00 1.00	97.94 97.99
70	1534	C2	NAG A	340	39.952	-9.673	19.363	1.00	100.93 110.08

	1535	N2	NAG A	340	39.319	-10.976	19.455	4 00	404
	1536	C7	NAG A	340	39.582	-11.912	18.542	1.00	124.78
	1537	07 ·	NAG A	340	40.340	-11.731	17.581	1.00. 1.00	135.15
_	1538	C8	NAG A	340	38.887	-13.255	18.716	1.00	143.28
5	1539	cs	NAG A	340	41.289	-9.672	20.154	1.00	133.94
	1540	03	NAG A	340	42.244	-10.545	19.553	1.00	111.41 102.38
	1541	C4	NAG A	340	41.892	-8.253	20.277	1.00	118.52
	1542	04	NAG A	340	42.980	-8.268	21.194	1.00	138.80
10	1543	C5	NAG A	340	40.818	-7.251	20.750	1.00	112.80
10	1544	05	NAG A	340	39.674	-7.325	19.890	1.00	95.92
	1545	C6	NAG A	340	41.276	-5.810	20.749	1.00	115.39
	1546	06	NAG A	340	40.167	-4.937	20.919	1.00	113.34
	1547	C1	NAG A	366	26.559	-8.481	-3.518	1.00	137.03
15	1548	C2	NAG A	366	25.744	-9.77 1	-3.450	1.00	148.09
13	1549	N2	NAG A	366	26.028	-10.464	-2.209	1.00	155.02
	1550	C7	NAG A	366	25.085	-10.564	-1.276	1.00	162.56
	1551 1552	O7	NAG A	366	23.951	-10.097	· -1.415	1.00	164.09
	1553	C8 C3	NAG A	366	25.455	-11.299	0.005	1.00	163.28
20	1554	03	NAG A	366	26.084	-10.660	-4.651	1.00	155.95
20	1555	C4	NAG A NAG A	366	25.247	-11.807	-4.658	1.00	159.81
	1556	04	NAG A	366	25.893	-9.878	-5.955	1.00	160.49
	1557	C5	NAG A	366 366	26.355	-10.659	-7.048	1.00	169.57
	1558	O5	NAG A	366	26.666	-8.550	-5.904	1.00	155.12
25	1559	C6	NAG A	366	26.272	-7.789 7.770	-4.739	1.00	140.93
	1560	O6	NAG A	366	26.413	-7.679 6.264	-7.123	1.00	152.76
	1561	CB	VAL B	1	26.023 4.75≿	-6.364 40.855	-6.753	1.00	149.51
	1562	CG1	VAL B	i	5.003	40.880	51.137	1.00	126.57
	1563	CG2	VAL B	i	3.866	42.021	49.633	1.00	131.97
30	1564	c	VAL B	i	5.086	38.381	51.535 51.284	1.00	130.09
	1565	Ō	VAL B	i	6.179	38.608	50.764	1.00 1.00	100.44
	1566	N	VAL B	1	3.657	39.534	52.971	1.00	97.65
	1567	CA	VAL B	1	4.091	39.511	51.550	1.00	122.36 110.89
~=	1568	N	PRO B	2	4.743	37.150	51.681	1.00	91.57
35	1569	CD	PRO B	2	3.715	36.682	52.617	1.00	86.81
	1570	CA	PRO B	2	5.701	36.083	51.401	1.00	92.03
	1571	C8	PRO B	2	5.219	34.937	52.280	1.00	92.13
	1572	ÇG	PRO B	2	4.469	35.618	53.356	1.00	98.41
40	1573	C	PRO B	2	5.482	35.783	49.928	1.00	104,42
40	1574	0	PRO B	2	4.381	35.956	49.405	1.00	108.80
	1575	N	GLN B	3	6.522	35.337	49.251	1.00	115.31
	1576 1577	CA CB	GLN B	3	6.395	35.044	47.839	1.00	118.75
	1578	CG	GLN B	3	7.319	35.945	47.050	1.00	132.23
45	1579	CD	GLN B GLN B	3	6.978	37.381	47.261	1.00	134.41
	1580	OE1	GLN B	3	5.850	37.837	46.374	1.00	126.94
	1581	NE2	GLN B	3 3	4.815 6.038	37.173 38.982	46.271	1.00	124.90
	1582	C	GLN B	3	6.793	33.624	45.724	1.00	122.46
	1583	ŏ	GLN B	3	7.983	33.320	47.639	1.00	113.83
50	1584	Ň	LYS B	4	5.812	32.736	47.488 47.641	1.00	116.50
	1585	CA	LYS B	4	6.188	31.357	47.465	1.00 1.00	104.77
	1586	СВ	LYS B	4	4.972	30.448	47.319	1.00	92.78
	1587	CG	LYS B	4	3.816	31.031	46.558	1.00	100.70
	1588	CD	LYS B	4	2.912	29.900	46.094	1.00	119.63 129.60
55	1589	CE	LYS B	4	1.591	30.427	45.556	1.00	131.81
	1590	NZ	LYS B	4	0.528	29.403	45.762	1.00	129.85
	1591	С	LYS B	4	7.093	31.230	46.253	1.00	81.27
	1592	0	LYS B	4	6.904	31.908	45.239	1.00	74.91
60	1593	N	PRO B	5	8.133	30.392	46.370	1.00	75.63
60	1594	CD	PRO B	5	8.529	29.619	47.557	1.00	71.19
	1595	CA	PRO B	5	9.074	30.177	45.271	1.00	65.65
	1596	CB	PRO B	5	10.020	29.110	45.820	1.00	54.74
	1597	ÇG	PRO B	5	9.982	29.343	47.268	1.00	65.46
65	1598	C	PRO B	5	8.255	29.650	44.097	1.00	64.33
U.J	1599 1600	0	PRO B	5	7.090	29.277	44.255	1.00	65.82
	1600	N	LYS B	6	8.858	29.608	42.923	1.00	65.65
	1602	CA CB	LYS B Lys b	6	8.152	29.109	41.762	1.00	62.04
	1603	CG	LYS B	6	7.636	30.279	40.927	1.00	55.18
70	1604	CD	LYS B	6 6	6.697 5.394	29.866	39.817	1.00	89.38
. •			E. G D	v	5.594	30.661	39.855	1.00	97.54

	1605 1606	CE NZ	LYS B	6	4.431	30.196	38.756	1.00	92.63
	1607	NZ C	LYS B LYS B	6	3.107	30.872	38.837	1.00	79.21
	1608	ŏ	LYS B	6 6	9.121	28.262	40.961	1.00	65.56
5	1609	Ň	VAL B	7	10.042 8.931	28.789 26.946	40.325	1.00	67.90
-	1610	CA	VAL B	7	9.803	26.041	41.015 40.280	1.00	70.60
	1611	СВ	VAL B	7	9.507	24.560	40.595	1.00 1.00	65.28
	1612	CG1	VAL B	7	10.356	23.663	39.694	1.00	57.35
10	1613	CG2	VAL B	7	9.806	24.266	42.064	1.00	39.82 63.76
10	1614	C	VAL B	7	9.621	26.268	38.785	1.00	60.19
	1615	0	VAL B	7	8.498	26.325	38.280	1.00	56.68
	1616 1617	N CA	SER B	8	10.736	26.423	38.087	1.00	44.71
	1618	CB	SER B SER B	8 8	10.719	26.639	36.656	1.00	31.26
15	1619	OG OG	SER B	8	11.396 12.802	27.952	36.318	1.00	41.26
	1620	č	SER B	8	11.540	27.750 25.504	36.214	1.00	38.80
	1621	Ō	SER B	8	12.480	25.002	36.055 36.675	1.00 1.00	48.76
	1622	N	LEU B	9	11.202	25.094	34.844	1.00	52.73 48.97
00	1623	CA	LEU B	9	11.947	24.009	34.225	1.00	39.06
20	1624	СВ	LEU B	9	11.000	22.902	33.735	1.00	33.73
	1625	CG	LEU B	9	9.752	22.521	34.533	1.00	40.03
	1626	CD1	LEU B	9	9.198	21.252	33.933	1.00	39.96
	1627 1628	CD2 C	LEU B	9 9	10.071	22.302	35.993	1.00	58.00
25	1629	ŏ	LEU B	9	12.764 12.353	24.506	33.041	1.00	33.09
	1630	Ň	ASN B	10	13.930	25.413 23.908	32.317	1.00	31.06
	1631	ĊA	ASN B	10	14.768	24.262	32.848 31.721	1.00	19.95
	1632	CB	ASN B	10	15.833	25.276	32.096	1.00 1.00	20.51 41.33
20	1633	CG	ASN B	10	16.763	25.559	30.942	1.00	52.07
30	1634	OD1	ASN B	10	16.325	26.031	29.890	1.00	83.63
	1635	ND2	ASN B	10	18.048	25.263	31.119	1.00	49.68
	1636 1637	C	ASN B	10	15.446	23.008	31.211	1.00	34.87
	1638	O N	ASN B PRO B	10	16.375	22.497	31.843	1.00	40.39
35	1639	CD	PRO B	11 11	15.025 15.817	22.518	30.034	1.00	43.40
- •	1640	CA	PRO B	11	13.956	21.532 23.087	29.277 29.197	1.00	30.44
	1641	CB	PRO B	11	14.085	22.307	27.918	1.00 1.00	20.84 36.80
	1642	CG	PRO B	11	15.604	21.988	27.879	1.00	28.71
40	1643	Č	PRO B	11	12.572	22.964	29.819	1.00	34.02
40	1644	0	PRO B	11	12.312	22.023	30.566	1.00	49.37
	1645 1646	N	PRO B	12	11.663	23.896	29.482	1.00	30.69
	1647	CD CA	PRO B PRO B	12	11.938	24.837	28.384	1.00	30.68
	1648	CB	PRO B	12 12	10.268 9.668	24.026	29.945	1.00	24.81
45	1649	CG	PRO B	12	10.861	25.062 25.893	28.995	1.00	34.63
	1650	Č	PRO B	12	9.452	25.593 22.761	28.607 29.981	1.00 1.00	49.64
	1651	0	PRO B	12	8.465	22.654	30.716	1.00	29.55 28.29
	1652	N	TRP B	13	9.873	21.802	29.176	1.00	38.99
50	1653	CA	TRP B	13	9.188	20.527	29.057	1.00	44.73
50	1654	CB	TRP B	13	9.904	19.706	27.996	1.00	44.13
	1655 1656	CG CD2	TRP B	13	10.282	20.578	26.874	1.00	32.01
	1657	CE2	TRP B	13	9.428	21.507	26.210	1.00	33.06
	1658	CE3	TRP B	13 13	10.213	22.177	25.247	1.00	37.35
55	1659	CD1	TRP B	13	8.069 11.520	21.841 20.712	26.335	1.00	32.11
	1660	NE1	TRP B	13	11.487	21.675	26.306 25.330	1.00 1.00	30.68
	1661	· CZ2	TRP 8	13	9.686	23.160	24.411	1.00	32.77 42.92
	1662	CZ3	TRP B	13	7.545	22.816	25.507	1.00	36.94
60	1663	CH2	TRP B	13	8.354	23.466	24.553	1.00	51.15
UU	1664 1665	C	TRP B	13	9.079	19.747	30.356	1.00	42.74
	1666	0 N	TRP B ASN B	13	10.070	19.236	30.866	1.00	27.87
	1667	CA	ASN B	14	7.862	19.660	30.879	1.00	39.20
	1668	CB	ASN B	14 14	7.609 6.354	18.933	32.107	1.00	42.44
65	1669	ČĠ	ASN B	14	5.119	19.469 19.130	32.774 33.010	1.00	50.46
	1670	OD1	ASN B	14	4.967	19.509	32.010 30.852	1.00	49.15
	1671	ND2	ASN B	14	4.221	18.402	30.652 32.649	1.00 1.00	79.01 57.00
	1672	C	ASN B	14	7.427	17.455	31.790	1.00	57.09 43.98
70	1673	0	ASN B	14	7.263	16.635	32.683	1.00	61.67
70	1674	N	ARG B	15	7.443	17.126	30.507	1.00	44.77

	1675	CA	ARG B	15	7.293	15.749	30.065	1.00	37.62
	1676	CB	ARG B	15	6.053	15.588	29.197	1.00	37.62
	1677	CG	ARG B	15	4.972	16.603	29.455	1.00	44.80
5	1678 1679	CD	ARG B	15	3.826	16.330	28.510	1.00	56.59
,	1680	NE CZ	ARG B ARG B	15	3.226	15.032	28.791	1.00	41.31
	1681	NH1	ARG B	15 15	2.570	14.311	27.883	1.00	40.12
	1682	NH2	ARG B	15	2. 43 5 2.033	14.759	26.639	1.00	57.43
	1683	C	ARG B	15	8.522	າວ. ເວີ5 15. 500	28.246 29.221	1.00	28.82
10	1684	Ö	ARG B	15	8.737	16.159	28.202	1.00 1.00	31.33
	1685	N	ILE B	16	9.328	14.535	29.621	1.00	34.58
	1686	CA	ILE B	16	10.540	14.286	28.872	1.00	29.80 46.54
	1687	CB	ILE B	16	11.728	14.912	29.604	1.00	56.61
15	1688	CG2	ILE B	16	11.405	16.370	29.923	1.00	58.31
13	1689 1690	CG1 CD1	ILE B	16	11.988	14.150	30.9- 2	1.00	61.86
	1691	C	ILE B	16	13.106	14.716	31.753	1.00	58.95
	1692	ŏ	ILE B	16 16	10.813 10.303	12.811	28.652	1.00	43.09
	1693	Ň	PHE B	17	11.619	11.952 12.532	29.383 27.634	1.00	46.04
20	1694	CA	PHE B	17	12.001	1:67	27.303	1.00	34.79
	1695	CB	PHE B	17	12.605	11.118	25.894	1.00 1.00	46.60
	1696	CG	PHE B	17	11.585	11.032	24.793	1.00	38.91 49.23
	1697	CD1	PHE B	17	11.845	11.607	23.549	1.00	47.72
25	1698	CD2	PHE B	17	10.387	10.354	24.982	1.00	39.73
25	1699	CE1	PHE B	17	10.931	11.520	22.512	1.00	39.05
	1700 1701	CE2 CZ	PHE B	17	9.465	10.258	23.957	1.00	33.44
	1702	C	PHE B PHE B	17 17	9.736	10.840	22.713	1.00	50.08
	1703	ŏ	PHE B	17	13.028 13.828	10.639	28.305	1.00	53.02
30	1704	Ň	LYS B	18	12.996	11.405 9.330	28.859 28.536	1.00	46.68
	1705	CA	LYS B	18	13.942	8.691	29.439	1.00 1.00	49.36
	1706	CB	LYS B	18	13.694	7.183	29.470	1.00	46.09 30.09
	1707	CG	LYS B	18	14.791	6.380	30.134	1.00	62.01
35	1708	CD	LYS B	18	14.541	4.890	29.967	1.00	69.67
33	1709	CE	LYS B	18	15.591	4.051	30.696	1.00	79.54
	1710 1711	NZ C	LYS B Lys b	18	16.966	4.233	30.147	1.00	74.39
	1712	ŏ	LYS B	18 18	15.363 15.641	8.964	28.946	1.00	45.81
	1713	Ň	GLY B	19	16.261	8.877 9.305	27.761	1.00	48.24
40	1714	CA	GLY B	19	17.634	9.564	29.860 29.470	1.00 1.00	54.24
	1715	С	GLY B	19	17.942	11.011	29.142	1.00	48.03 57.65
	1716	0	GLY B	19	19.110	11.364	28.964	1.00	57.96
	1717	N	GLU B	20	16.916	11.855	29.050	1.00	59.66
45	1718	CA	GLU B	20	17.142	13.269	28.754	1.00	58.50
73	1719 1720	CB CG	GLU B GLU B	20	15.900	13.889	28.106	1.00	70.52
	1721	CD	GLU B	20 20	15.444 14.502	13.180	26.834	1.00	82,41
	1722	OE1	GLU B	20	13.490	14.026 14.527	25.992 26.550	1.00	79.78
	1723	OE2	GLU B	20	14.786	14.176	26.550 24.776	1.00 1.00	67.98
50	1724	С	GLU B	20	17.474	14.021	30.046	1.00	80. 7 5 52.56
	1725	0	GLU B	20	17. 26 6	13.492	31.143	1.00	35.18
	1726	N	ASN B	21	17.999	15.244	29.920	1.00	59.52
	1727	CA	ASN B	21	18.344	16.072	31.085	1.00	47.35
55	1728 1729	CB CG	ASN B	21	19.753	16.640	30.956	1.00	30.47
33	1730	OD1	ASN B ASN B	21	20.784	15.572	30.658	1.00	55.82
	1731	ND2	ASN B	21 21	20.688 21.772	14.447 15.924	31.168	1.00	46.16
	1732	C	ASN B	21	17.383	17.239	29.835 31.261	1.00	67.36
	1733	0	ASN B	21	16.866	17.784	30.292	1.00 1.00	40.95 70.03
60	1734	N	VAL B	22	17.152	17.619	32.507	1.00	25.27
	1735	CA	VAL B	22	16.276	18.735	32.829	1.00	32.44
	1736	CB	VAL B	22	14.824	18.247	33.003	1.00	20.08
	1737 1738	CG1	VAL B	22	14.692	17.429	34.270	1.00	24.18
65	1739	CG2 C	VAL B	22	13.882	19.426	33.061	1.00	36.02
	1740	ŏ	VAL B VAL B	22 22	16.775	19.385	34.139	1.00	43.21
	1741	Ň	THR B	23	17.327 16.583	18.710 20.689	35.003	1.00	49.24
	1742	CA	THR B	23	17.030	21.383	34.289 35.489	1.00	39.88
70	1743	CB	THR B	23	18.165	22.352	35.469 35.174	1.00 1.00	33.49 34.45
70	1744	OG1	THR B	23	19.216	21.655	34.493	1.00	42.02
						•			76.06

	1745	CG2	THR B	23	18.693	22.967	36.456	1.00	52.09
	1746	C .	THR B	23	15.931	22.190	36.167	1.00	43.19
	1747 1748	N	THR B LEU B	23	15.405	23.157	35.608	1.00	46.71
5	1749	CA	LEU B	24 24	15.591 14.581	21.797 22.521	37.383	1.00	44.29
_	1750	СВ	LEU B	24	13.911	21.596	38.131 39.141	1.00 1.00	54.45
	1751	CG	LEU B	24	13.237	20.376	38.519	1.00	48.21 51.83
	1752	CD1	LEU B	24	12.426	19.622	39.562	1.00	56.70
10	1753 1754	CD2	LEU B	24	12.329	20.835	37.415	1.00	69.70
10	1755	C	LEV B	24 24	15.255	23.676	38.858	1.00	60.50
	1756	Ň	THR B	2 4 25	16.299 14.669	23.494 24.865	39.482 38.771	1.00	84.20
	1757	CA	THR B	25	15.238	26.025	39.439	1.00 1.00	56.15
	1758	CB	THR B	25	15.715	27.055	38.435	1.00	48.18 36.73
15	1759	OG1	THR B	25	16.498	26.395	37.429	1.00	43.20
	1760 1761	CG2 C	THR B	25	16.584	28.095	39.134	1.00	58.01
	1762	ŏ	THR B	25 25	14.228 13.051	26.659 26.810	40.374	1.00	55.18
	1763	N	CYS B	26	14.700	27.010	40.019 41.571	1.00 1.00	39.05
20	1764	С.	CYS B	26	13.866	27.603	42.608	1.00	69.20 77.69
	1765	Ç	CYS B	26	14.115	29.091	42.752	1.00	84.84
	1766 1767	O CB	CYS B	26	15.186	29.501	43.193	1.00	95.13
	1768	SG	CYS B	26 26	14.146	26.925	43.947	1.00	70.99
25	1769	N	ASN B	27	12.878 13.127	27.161 29.898	45.240 42.378	1.00	87.46
	1770	CA	ASN B	27	13.234	31.349	42.491	1.00 1.00	94.31 97.02
	1771	CB	ASN B	27	14.182	31.917	41.409	1.00	104.76
	1772	CG	ASN B	27	13.616	31.796	39.988	1.00	106.25
30	1773 1774	OD1 ND2	ASN B ASN B	27	12.599	31.141	39.748	1.00	109.42
50	1775	C	ASN B	27 27	14.293 11.848	32.434	39.035	1.00	104.71
	1776	ŏ	ASN B	27	10.979	31.975 31,462	42.388 41.684	1.00 1.00	95.21 83.43
	1777	N	GLY B	28	11.639	33.069	43.112	1.00	106.07
25	1778	CA	GLY B	28	10.354	33.753	43.101	1.00	127.70
35	1779 1780	C	GLY B	28	10.461	34.992	43.966	1.00	138.06
	1781	N	GLY B ASN B	28 29	10.631 10.341	34.879	45.182	1.00	143.08
	1782	CA	ASN B	29	10.498	36.173 37.424	43.362 44.099	1.00 1.00	142.87 153.48
40	1783	CB	ASN B	29	9.350	37.669	45.082	1.00	152.59
40	1784	CG	ASN B	29	9.535	38.959	45.876	1.00	158.12
	1785 1786	OD1 ND2	ASN B ASN B	29	10.508	39.679	45.675	1.00	156.21
	1787	C	ASN B	29 29	8.607 11.787	39.253 37.198	46.772	1.00	158.95
	1788	ŏ	ASN B	29	11.820	37.150	44.865 46.094	1.00 1.00	161.65
45	1789	N	ASN B	30	12.842	36.920	44.109	1.00	164.05 173.43
	1790	CA	ASN B	30	14.136	36.629	44.690	1.00	183.92
	1791 1792	CB CG	ASN B	30	15.174	36.378	43.593	1.00	190.23
	1793	OD1	ASN B	30 30	16.451 16.552	35.752 35.442	44.136	1.00	197.43
50	1794	ND2	ASN B	30	17.431	35.555	45.325 43.262	1.00 1.00	203.09 200.85
	1795	Ç	ASN B	30	14.653	37.685	45.639	1.00	186.26
	1796	o :	ASN B	30	14.262	38.855	45.593	1.00	185.38
	1797 1798	N CA	PHE B	31	15.547	37.235	46.501	1.00	188.59
55	1799	CB	PHE B	31 31	16.173 15. 4 85	38.036 37.780	47.500	1.00	194.52
	1800	ČĠ	PHE B	31	15.971	38.766	48.8-\1 49.886	1.00 1.00	203.03
	1801	CD1	PHE B	31	15.408	40.027	49.940	1.00	210.47 216.06
	1802	CD2	PHE B	31	16.993	38.456	50.730	1.00	211.10
60	1803 1804	CE1 CE2	PHE B	31	15.861	40.961	50.804	1.00	222.00
00	1805	CZ	PHE B	31 31	17.485	39.387	51.600	1.00	215.51
	1806	č	PHE B	31	16.924 17.649	40.643 37.672	51.640	1.00	219.04
	1807	Ō	PHE B	31	18.344	37.980	47.559 48.535	1.00 1.00	191.71 197.27
65	1808	N	PHE B	32	18.115	36.994	46.528	1.00	183.37
65	1809	CA CB	PHE B	32	19.516	36.543	46.471	1.00	176.18
	1810 1811	CB CG	PHE B	32	20.457	37.696	46.108	1.00	171.85
	1812	CD1	PHE B	32 32	20.693 21.637	38.668 38.396	47.204 49.197	1.00	170.32
	1813	CD2	PHE B	32	19.977	39.859	48.187 47.276	1.00 1.00	169.89 168.03
70	1814	CE1	PHE B	32	21.868	39.298	49.221	1.00	164.25
									11100

	1815	CE2	PHE B	32-	20.201	40.765	48.308	1.00	160.78
	1816 1817	CZ C	PHE B PHE B	32	21.145	40.483	49.282	1.00	159.57
	1818	ŏ	PHE B	32 32	19.870 21.029	35.945 35.946	47.824	1.00	175.68
5	1819	N	GLU B	33	18.872	35.409	48. 23 5 48.474	1.00 1.00	173.43
	1820	CA	GLU B	33	19.012	34.712	49.721	1.00	177.15 177.13
	1821	CB	GLU B	33	17.859	35.035	50.674	1.00	177.13
	1822 1823	CG	GLU B	33	18.021	34.459	52.073	1.00	176.70
10	1824	CD OE1	GLU B	33 33	19.050	35.206	52.898	1.00	173.43
••	1825	OE2	GLU B	33	19.758 19.151	36.067 34.929	52.334 54.111	1.00	173.17
	1826	C	GLU B	33	18.966	33.237	49.329	1.00 1.00	172.06 175.21
	1827	0	GLU B	33	18.622	32.361	50.122	1.00	174.80
15	1828	N	VAL B	34	19.311	32.998	48.071	1.00	172.32
13	1829 1830	CA CB	VAL B VAL B	34	19.336	31.679	47.454	1.00	166.26
	1831	CG1	VAL B	34 34	20.040 20.242	31.769 30.393	46.083	1.00	167.66
	1832	CG2	VAL B	34	19.234	32.658	45.487 45.147	1.00 1.00	171.78
00	1833	С	VAL B	34	19.997	30.573	48.274	1.00	170.77 160.12
20	1834	0	VAL B	34	19.643	29.405	48.137	1.00	161.37
	1835	N	SER B	35	20.953	30.940	49.117	1.00	154.76
	1836 1837	CA CB	SER B SER B	35	21.668	29.962	49.933	1.00	144.31
	1838	OG OG	SER B	35 35	22.442 21.565	30.673 31.183	51.049	1.00	145.69
25	1839	č	SER B	35	20.772	28.897	52.038 50.555	1.00 1.00	143.47
	1840	0	SER B	35	21.184	27.749	50.708	1.00	136.95 135.37
	1841	N .	SER B	36	19.547	29.269	50.912	1.00	130.67
	1842	CA	SER B	36	18.623	28.328	51.542	1.00	127.00
30	1843 1844	CB OG	SER B	36	17.944	28.990	52.748	1.00	133.26
50	1845	C	SER B SER B	36 36	17.047 17.545	30.017	52.345	1.00	123.80
	1846	ŏ	SER B	36	16.620	27.766 28.481	50.615 50.222	1.00 1.00	123.00
	1847	N	THR B	37	17.657	26.480	50.282	1.00	128.61 107.86
25	1848	CA	THR B	37	16.675	25.821	49.426	1.00	88.91
35	1849	CB	THR B	37	17.089	25.793	47.928	1.00	87.15
	1850 1851	OG1 CG2	THA B THA B	37	17.358	27.116	47.445	1.00	64.20
	1852	C	THR B	37 37	15.955 16.469	25.213 24.376	47.103	1.00	90.90
	1853	Ö	THR B	37	17.427	23.669	49.854 50.168	1.00 1.00	86.86 83.90
40	1854	N	LYS B	38	15.212	23.948	49.845	1.00	82.11
	1855	CA	LYS B	38	14.835	22.596	50.224	1.00	83.86
	1856 1857	CB CG	LYS B LYS B	38	13.885	22.630	51.427	1.00	86.79
	1858	CD	LYS B	38 38	14.442 15.694	22.010	52.699	1.00	100.07
45	1859	ČE	LYS B	38	16.039	22.734 22.305	53.185 54.602	1.00 1.00	104.27
	1860	NZ	LYS B	38	14.882	22.578	55.510	1.00	97.90 91.89
	1861	Č	LYS B	38	14.115	21.953	49.051	1.00	82.06
	1862	0	LYS B	38	13.147	22.520	48.545	1.00	72.96
50	1863 1864	N CA	TRP B	39 39	14.579	20.784	48.613	1.00	82.25
50	1865	CB	TRP B	39	13.915 14.922	20.097 19.675	47.508	1.00	66.31
	1866	CG	TRP B	39	15.429	20.832	46.449 45.665	1.00 1.00	58.26 63.66
	1867	CD2	TRP B	39	14.789	21.453	44.542	1.00	65.27
55	1868	CE2	TRP B	39	15.607	22.534	44.139	1.00	67.87
22	1869 1870	CE3	TRP B	39	13.605	21,201	43.841	1.00	51.05
	1871	CD1 NE1	TRP B	39	16.574	21.541	45.891	1.00	62.46
	1872	CZ2	TRP B	39 39	16.690 15 <i>.2</i> 77	22.565 23.364	44.977	1.00	57.52
	1873	CZ3	TRP B	39	13.280	22.023	43.061 42.775	1.00 1.00	59.34 59.55
60	1874	CH2	TRP B	39	14.114	23.093	42.395	1.00	51.52
	1875	C	TRP B	39	13.113	18.888	47.971	1.00	57.60
	1876 1877	O N	TRP B	39	13.484	18.191	48.920	1.00	57.66
	1878	CA	PHE B PHE B	40 40	11.993	18.652	47.304	1.00	54.42
65	1879	CB	PHE B	40	11.149 9.926	17.534 18.018	47.671 48.449	1.00	62.19
	1880	CG	PHE B	40	10.262	18.678	48.449 49.745	1.00 1.00	54.85 59.54
	1881	CD1	PHE B	40	10.602	. 20.025	49.783	1.00	63.79
	1882	CD2	PHE B	40	10.310	17.934	50.920	1.00	65.98
70	1883 1884	CE1 CE2	PHE B	40	10.988	20.623	50.981	1.00	81.46
, ,	1007	CEZ	PHE B	40	10.696	18.518	52.122	1.00	72.69

	1885	CZ		400	44.000	42.222			
	1886	č	PHE B PHE B	40° 40	11.039 10.688	19.863 16.728	52.154	1.00	78.47
	1887	ō:	PHE B	40	9.920	17.217	46.476 45.650	1.00	68.64
` _	1888	N .	HIS B	41	11.157	15.487	46.396	1.00 1.00	78.19 72.46
5	1889	CA	HIS B	41	10.778	14.593	45.314	1.00	69.06
	1890 1891	CB CG	HIS B	41	11.988	13.804	44.833	1.00	61.71
	1892	CD2	HIS B HIS B	41 41	11.706	12.972	43.630	1.00	66.30
	1893	ND1	HIS B	41	12.491 10.476	12.132 12.970	42.921	1.00	62.70
10	1894	CE1	HIS B	41	10.517	12.161	43.011 41.967	1.00 1.00	68.58
	1895	NE2	HIS B	41	11.728	11.640	41.890	1.00	82.82 79.59
	1896	C	HIS B	41	9.713	13.641	45.839	1.00	66.17
	1897 1898	0 N	HIS B ASN B	41	9.971	12.842	46.727	1.00	64.30
15	1899	CA	ASN B	42 42	8.511 7.423	13.726 12.877	45.288	1.00	75.54
	1900	СВ	ASN B	42	7.739	11.397	45.751 45.530	1.00 1.00	79.71
	1901	CG	ASN B	42	7.203	10.871	44.210	1.00	78.21 78.51
	1902	OD1	ASN B	42	6.080	11.203	43.803	1.00	76.64
20	1903 1904	ND2	ASN B	42	8.001	10.027	43.560	1.00	77.12
20	1904	C	ASN B ASN B	42	7.183	13.113	47.236	1.00	79.13
	1906	Ň	GLY B	42 43	6.754 7.478	12.203	47.958	1.00	64.42
	1907	CA	GLY B	43	7.276	14.330 14.662	47.692 49.091	1.00	81.21
~-	1908	C	GLY B	43	8.459	14.460	50.020	1.00 1.00	80.48
25	1909	0	GLY B	43	8.452	14.985	51.123	1.00	64.04 63.95
	1910	N	SER B	44	5.472	. 13.719	49.573	1.00	59.76
	1911 1912	CA CB	SER B	44	10.655	13.449	50.387	1.00	64.76
	1913	OG OG	SER B SER B	44 44	11.191 10.248	12.034	50.114	1.00	70.69
30	1914	Č	SER B	44	11.758	11.045 14.454	50.502	1.00	89.71
	1915	Ö	SER B	44	12.038	14.802	50.134 48.993	1.00 1.00	65.31
	1916	N	LEU B	45	12.386	14.914	51.209	1.00	76.25 65.35
	1917	CA	LEU B	45	13.471	15.877	51.100	1.00	61.98
35	1918 1919	CB CG	LEU B	45	13.917	16.337	52.496	1.00	65.46
33	1920	CD1	LEV B LEV B	45 45	15.182	17.202	52.529	1.00	79.05
	1921	CD2	LEU B	45 45	14.971 15.526	18.471 17.548	51.691 53.071	1.00	77.35
	1922	C	LEU B	45	14.663	15.278	53.971 50.351	1.00 1.00	72.35 60.60
40	1923	0	LEU B	45	15.109	14.168	50.638	1.00	63.58
40	1924	N	SER B	46	15.167	16.015	49.374	1.00	61.57
	1925 1926	CA CB	SER B	46	16.315	15.564	48.608	1.00	73.03
	1927	OG	SER B SER B	46 46	16.247	16.120	47.186	1.00	<i>77.2</i> 2
	1928	č	SER B	46	17.386 17.569	15. 7 37 16.083	46.432 49.302	1.00	90.60
45	1929	0	SER B	46	17.499	16.999	50.129	1.00 1.00	80.37 76.01
	1930	N	GLJ B	47	18.710	15.493	48.969	1.00	84.85
	1931	CA	GLU B	47	19.974	15.930	49.548	1.00	84.12
	1932 1933	CB CG	GLU B	47	21.027	14.827	49.429	1.00	87.82
50	1934	CD	GLU B GLU B	47 47	20.659	13.538	50.145	1.00	101.06
	1935	OE1	GLU B	47	20.468 20.638	13.733 14.876	51. 637 52.113	1.00	111.75
	1936	OE2	GLU B	47	20.148	12.744	52.329	1.00 1.00	115.76
	1937	С	GLU B	47	20.468	17.212	48.886	1.00	12.59 82.4 2
55	1938	0	GLU B	47	21.259	17.951	49.455	1.00	91.17
JJ	1939 1940	N	GLU B	48	19.971	17.458	47.675	1.00	78.36
	1941	CA CB	GLU B	48	20.339	18.649	46.918	1.00	77.76
	1942	ca	GLU B	48 48	19.624 19.932	18.652 19.876	45.569	1.00	83.13
	1943	CD	GLU B	48	21.376	19.914	44.726 44.265	1.00 1.00	92.74
60	1944	OE1	GLU B	48	21.677	19.317	43.203	1.00	101.93 102.91
	1945	OE2	GLU B	48	22.204	20.531	44.975	1.00	108.55
	1946 1947	C	GLU B	48	19.970	19.916	47.686	1.00	77.31
	1947	O N	GLU B THR B	48 40	18.853	20.040	48.204	1.00	74.82
65	1949	CA	THR B	49 49	20.900 20.659	20.864	47.749	1.00	78.12
	1950	CB	THR B	49	21.526	22,107 22,184	48.475 49.748	1.00 1.00	81.85
	1951	OG1	THR B	49	22.684	21.353	49.593	1.00	83.91 88.24
	1952	CG2	THR B	49	20.726	21.743	50.961	1.00	75.28
70	1953 1954	C	THR B	49	20.871	23.390	47.680	1.00	82.91
70	1954	0	THR B	49	20.664	. 24.481	48.208	1.00	84.53

	1955 1956	N CA	ASN B ASN B	50°	21.296	23.273	46.425	1.00	89.01
	1957	CB	ASN B	50 50	21.491	24.455	45.592	1.00	90.45
	1958	CG	ASN B	50 50	22.483 22.910	24.139 25.375	44.463	1.00	96.17
5	1959	OD1	ASN B	50	22.449	26.482	43.697 43.971	1.00	111.81
	1960	ND2	ASN B	50	23.798	25.190	42.727	1.00 1.00	112.79
	1961	С	ASN B	50	20.123	24.856	45.013	1.00	110.81 89.21
	1962	0	ASN B	50	19.208	24.033	44.942	1.00	94.63
10	1963	N	SER B	51	19.976	26.118	44.625	1.00	84.28
10	1964	CA	SER B	51	18.724	26.613	44.045	1.00	84.66
	1965 1966	CB OG	SER B	51	18.820	28.123	43.846	1.00	90.77
	1967	Č	SER B SER B	51 51	20.000 18.387	28.461	43.134	1.00	104.30
	1968	ŏ	SER B	51	17.312	25.940 26.150	42.699 42.126	1.00	77.58
15	1969	Ň	SER B	52	19.313	25.133	42.195	1.00 1.00	52.63
	1970	CA	SER B	52	19.108	24.441	40.934	1.00	74.45 62.55
	1971	CB	SER B	52	20.120	24.930	39.907	1.00	56.77
	1972	og	SER B	52	20.003	26.329	39.742	1.00	76.18
20	1973 1974	C	SER B	52	19.243	22.934	41.098	1.00	61.53
20	1975	0 N	SER B LEU B	52	20.327	22.425	41.391	1.00	66.28
	1976	CA	LEU B	53 53	18.133 18.102	22.229	40.915	1.00	56.00
	1977	CB	LEU B	53	16.789	20.778 20.323	41.014	1.00	42.82
	1978	CG	LEU B	53	16.530	18.816	41.642 41.653	1.00 1.00	35.21
25	1979	CD1	LEU B	53	17.775	18.057	42.111	1.00	46.47 51.40
	1980	CD2	LEU B	53	15.337	18.539	42.565	1.00	29.95
	1981	C	LEU B	53	18.236	20.189	39.627	1.00	40.92
	1982 1983	0	LEU B	53	17.347	20.338	38.801	1.00	59.69
30	1984	N CA	ASN B ASN B	54	19.353	19.524	39.372	1.00	53.72
20	1985	CB	ASN B ASN B	54 54	19.593 21.064	18.921	38.068	1.00	63.37
	1986	ČĞ	ASN B	54	21.475	19.074 20.516	37.686 37.562	1.00	66.79
	1987	OD1	ASN B	54	20.985	21.239	36.691	1.00 1.00	81.16 89.84
~~	1988	ND2	ASN B	54	22.372	20.952	38.439	1.00	99.57
35	1989	С	ASN B	54	19.205	17.444	37.989	1.00	68.27
	1990	0	ASN B	54	19.398	16.681	38.935	1.00	72.52
	1991	N	ILE B	55	18.643	17.061	36.849	1.00	66.50
	1992 1993	CA CB	ILE B	55 55	18.242	15.689	36.596	1.00	55.12
40	1994	CG2	ILE B	55 55	16.744 16.431	15.574	36.310	1.00	34.50
	1995	CG1	ILE B	· 55	15.952	14.175 15.909	35.822 37.577	1.00	22.09
	1996	CD1	ILE B	55	14.466	15.688	37.459	1.00 1.00	32.78 38.73
	1997	С	ILE B	55	19.012	15.235	35.371	1.00	57.07
45	1998	0	ILE B	55	18.806	15.751	34.276	1.00	69.88
45	1999	N	VAL B	56	19.910	14.277	35.560	1.00	58.62
	2000 2001	CA	VAL B	56	20.719	13.795	34.450	1.00	65.98
	2001	CB CG1	VAL B VAL B	56 56	22.202	13.797	34.826	1.00	58.88
	2003	CG2	VAL B VAL B	56 56	23.047 22.573	13.490	33.609	1.00	54.44
50	2004	C	VAL B	56	∠0.326	15.146 12.401	35.401 33.984	1.00	58.22
	2005	ō	VAL B	56	20.232	11.468	34.782	1.00 1.00	71.96 82.07
	2006	N	ASN B	57	20.103	12.272	32.678	1.00	70.61
	2007	CA	ASN B	57	19.704	11.006	32.081	1.00	79.87
55	2008	CB	ASN B	57	20.879	10.028	32.084	1.00	88.09
33	2009	CG	ASN B	57	22.082	10.573	31.331	1.00	104.06
	2010 2011	OD1	ASN B	57	21.990	10.934	30.151	1.00	109.39
	2012	ND2 C	ASN B ASN B	57 57	23.220 18.532	10.640	32.013	1.00	110.76
	2013	ŏ	ASN B	57 57	18.597	10.441 9.335	32.865	1.00	77.25
60	2014	Ň	ALA B	58	17.463	11.229	33.403 32.916	1.00 1.00	83.22 69.58
	2015	CA	ALA B	58	16.246	10.872	33.629	1.00	67.83
	2016	CB	ALA B	58	15.101	11.748	33.155	1.00	70.80
	2017	Ç	ALA B	58	15.854	9.399	33.519	1.00	66.71
65	2018	0	ALA B	58	15.912	8.790	32.455	1.00	63.76
UJ	2019	N	LYS B	59	15.472	8.837	34.655	1.00	62.18
	2020 2021	CA	LYS B	59 50	15.035	7.452	34.742	1.00	62.15
	2022	CB CG	LYS B LYS B	59 59	15.688	6.774	35.943	1.00	77.31
	2023	CD	LYS B	59 59	17.214 17.816	6.849 6.471	35.933 37.977	1.00	89.39
70	2024	CE	LYS B	59	19.320	6.717	37.277 37.280	1.00	86.69 83.05
						G., 17	J. 200	1.00	83.05

	2025	. NZ	LYS B	59	10.014	0.500			
	2026	С	LYS B	59	19.914 13.548	6.523 7.589	38.630 34.978	1.00	80.45
	2027 2028	0	LYS B	59	13.062	8.707	35.128	1.00 1.00	56.91
5	2029	N CA	PHE B	60	12.813	6.486	35.016	1.00	72.49 42.51
_	2030	CB	PHE B	60 60	11.380 10.657	6.608	35.244	1.00	48.10
	2031	CG	PHE B	60	10.808	5.310 4.884	34.915	1.00	48.50
	2032	CD1	PHE B	60	11.919	4.149	33.480 33.072	1.00 1.00	64.06
10	2033 2034	CD2 CE1	PHE B	60	9.837	5.216	32.533	1.00	63.95 74.15
••	2035	CE2	PHE B PHE B	60	12.068	3.753	31.739	1.00	62.10
	2036	CZ	PHE B	60 60	9.977 11.092	4.826 4.089	31.196	1.00	74.92
	2037	Ç	PHE B	60	11.166	6.962	30.801 . 6.693	1.00	69.78
15	2038 2039	0	PHE B	60	10.203	7.639	67.058	1.00 1.00	55.02
13	2040	N CA	GLU B GLU B	61	12.097	6.503	37.517	1.00	61.86 75.45
	2041	CB	GLU B	61 61	12.044 13.190	6.763	38.944	1.00	83.97
	2042	CG	GLU B	61	13.190	6.038 4.505	39.668	1.00	96.33
20	2043	CD	GLU B	61	13.368	3.847	39.705 38.362	1.00 1.00	106.00
20	2044 2045	OE1 OE2	GLU B	61	14.506	3.988	37.861	1.00	110.30 109.44
	2046	C	GLU B GLU B	61 61	12.459	3.187	37.811	1.00	111.21
	2047	Ō	GLU B	61	12.136 11.814	8.267 8.747	39.188	1.00	78.63
25	2048	N	ASP B	62	12.579	9.007	40.277 [*] 38.174	1.00	79.41
45	2049 2050	CA	ASP B	62	12.698	10.452	38.299	1.00 1.00	64.96 56.09
	2051	CB CG	ASP B ASP B	62	13.720	11.010	37.306	1.00	58.67
	2052	OD1	ASP B	62 62	15.152 15.467	10.763	37.744	1.00	72.63
30	2053	OD2	ASP B	62	15.963	11.068 10.277	38.916 36.923	1.00	85.98
30	2054 2055	C	ASP B	62	11.366	11.151	38.094	1.00 1.00	71.52 52.65
	2056	0 N	ASP B SER B	62	11.227	12.325	38.442	1.00	52.65 50.83
	2057	CA	SER B	63 63	10.391	10.440	37.533	1.00	47.35
25	2058	СВ	SER B	63	9.076 8.157	11.029 10.038	37.311	1.00	51.69
35	2059	og	SER B	63	8.676	9.676	36.609 35.341	1.00 1.00	59.14
	2060 2061	C	SER B	63	8.511	11.353	38.669	1.00	76.77 48.98
	2062	Ň	SER B GLY B	63 64	9.048	10.900	39.666	1.00	55.63
40	2063	CA	GLY B	64	7.439 6.846	12.135 12.460	38.717	1.00	50.75
40	2064	C	GLY B	64	6.550	13.922	39.998 40.254	1.00 1.00	54.90
	2065 2066	0	GLY B	64	6.405	14.721	39.327	1.00	57.89 65.67
	2067	N CA	GLU B GLU B	65 65	6.456	14.260	41.536	1.00	63.70
	2068	CB	GLU B	65 65	6.161 5.036	15.619 15.576	41.982	1.00	62.19
45	2069	CG	GLU B	65	4.715	15.576 16.899	43.009 43.646	1.00	58.85
	2070 2071	CD	GLU B	65	3.957	16.719	44.960	1.00 1.00	74.39 96.38
	2072	OE1 OE2	GLU B GLU B	65 65	4.578	16.285	45.968	1.00	90.14
	2073	c	GLU B	65 65	2. 73 4 7.386	17.002	44.976	1.00	104.83
50	2074	0	GLU B	65	8.084	16.301 15.716	42.598 43.424	1.00	58.45
•	2075 2076	N	TYR B	66	7.647	17.533	42.176	1.00 1.00	57.76 49.99
	2077	CA CB	TYR B	66	8.768	18.291	42.696	1.00	34.15
	2078	ça	TYR B	66 66	9. 7 97 10.595	18.547	41.614	1.00	10.05
55	2079	CD1	TYR B	66	10.385	17.338 16.517	41.213	1.00	33.40
	2080	CE1	TYR B	66	10.957	15.427	40.173 39.766	1.00 1.00	44.01
	2081 2082	CD2 CE2	TYR B	66	11.794	17.042	41.841	1.00	55.60 51.50
	2083	CZ	TYR B TYR B	66 66	12.574	15.951	41.445	1.00	59.78
60	2084	OH	TYR B	66 66	12.154 12.927	15.150 14.073	40.405	1.00	62.67
	2085	Č	TYR B	66	8.311	19.623	40.013 43.246	1.00	60.36
	2086 2087	O	TYR B	66	7.440	20.275	42.671	1.00 1.00	44.11 50.42
	2088	N CA	LYS B Lys b	67 67	8.888	20.006	44.380	1.00	55.20
65	2089	CB	LYS B	67 67	8.577 7.289	21. <i>2</i> 75	45.043	1.00	54.38
	2090	CG	LYS B	67	7.289 7.088	21.199 19.925	45.879 48.675	1.00	37.10
	2091 2092	CD	LYS B	67	5.836	20.053	46.675 47.546	1.00 1.00	40.24
	2092	CE NZ	LYS B LYS B	67	5.362	18.702	48.076	1.00	55.82 71.24
70	2094	C	LYS B	67 67	4.355 9.725	18.855	49.172	1.00	79.55
					J.123	21.684	45.931	1.00	61.59

	2095	0	LYS B	67	10.222	20.891	46 700		
	2096 2097	N	CYS B	68	10.161	22.924	46.730 45.761		80.11
	2097	CA: C	CYS B	68	11.261	23.443	46.547		69.06
	5 2099	ŏ	CYS B	68	10.728	24.348	47.641		75.09
•	2100	СВ	CYS B	68	9.543	24.682	47.671	1.00	76.08
	2101	SG	CYS B	68	12.231	24.217	45.665	1.00	78.03
	2102	N	GLN B	68	11.523	25.691	44.866	1.00	71.35
	2103	ĊA	GLN B	69	11.625	24.756	48.527	1.00	75.66
10	2104	CB	GLN B	69	11.233	25.600	49.635	1.00	80.08 74.62
	2105	CG	GLN B	69 69		24.728	50.712	1.00	74.02 70.96
	2106	CD	GLN B	69	10.067 9.343	25.488	51.859	1.00	72.60
	2107	OE1	GLN B	69	9.406	24.592	52.818	1.00	88.38
1.6	2108	NE2	GLN B	69	8.656	23.363	52.720	1.00	85.19
15		С	GLN B	69	12.418	25.199 26.356	53.760	1.00	98.27
	2116	0	GLN B	69	13.519	25.819	50.212	1.00	78.27
	2111	N	HIS B	70	12.193	27.611	50.311	1.00	81.84
	2112	CA	HIS B	70	13.252	28.39ຄ	50.577	1.00	82.10
20	2113 2114	CB	HIS B	70	13.822	29.437	51.183 50.192	1.00	85.15
20	2115	CD2	HIS B	70	12.892	30.565	49.860	1.00	82.03
	2116	ND1	HIS B	70	12.763	31.800	50.398	1.00 1.00	93.26
	2117	CE1	HIS B HIS B	70	11.997	30.515	48.812	1.00	95.48
	2118	NE2		70	11.361	31.671	48.721	1.00	109.66
25	2119	C	HIS B HIS B	70	11.804	32.468	49.672	1.00	109.26 109.02
	2120	ŏ	HIS B	70	12.735	29.044	52.469	1.00	85.57
	2121	Ň	GLN B	70 71	11.549	29.350	52.598	1.00	85.74
	2122	CA	GLN B	71	13.635	29.213	53.431	1.00	79.77
20	2123	CB	GLN B	71	13.312 14.619	29.777	54.740	1.00	80.82
30	2124	CG	GLN B	71	14.460	30.126	55.465	1.00	89.59
•	2125	CD	GLN B	71	15.762	30.447 30.921	56.945	1.00	103.30
	2126	OE1	GLN B	71	16.789	30.220	57.585	1.00	109.00
	2127	NE2	GLN B	71	15.726	32.120	57.542 50.404	1.00	100.56
35	2128 2129	C	GLN B	71	12.365	30.993	58.184 54.763	1.00	102.47
33	2130	0	GLN B	71	12.486	31.913	53.953	1.00	67.00
	2131	N GA	GLN B	72	11.432	30.978	55.715	1.00	42.78
	2132	CB	GLN B	72	10.460	32.063	55.922	1.00 1.00	69.70
	2133	ČĠ	GLN B GLN B	72	11.188	33.388	56.149	1.00	70.51
40	2134	CD	GLN B	72	11.812	33.551	57.509	1.00	78.43 78.98
	2135	OE1	GLN B	72 70	12.598	34.838	57.593	1.00	95.13
	2136	NE2	GLN B	72 72	13.532	35.065	56.807	1.00	97.37
	2137	C	GLN B	72	12,223	35.700	58. 54 0	1.00	98.58
45	2138	0	GLN B	72	9.398 8.737	32.282	54.840	1.00	66.32
45	2139	N	VAL B	73	9.227	33.329	54.816	1.00	61.96
	2140	CA	VAL B	73	8.249	31.302 31.414	53.960	1.00	63.38
	2141	СВ	VAL B	73	8.933	31.810	52.884	1.00	57.15
	2142	CG1	VAL B	73	9.710	30.646	51.592	1.00	31.26
50	2143 2144	CG2	VAL B	73	7.918	32.256	51.074	1.00	36.55
50	2145	C	VAL B	73	7.552	30.075	50.585 52.663	1.00	50.56
	2146	0	VAL B	73	8.148	29.022	52.896	1.00	59.51
	2147	N CA	ASN B	74	6.300	30.115	52.210	1.00 1.00	77.00
	2148	CB	ASN B	74	5.534	28.892	51.965	1.00	61.46
55	2149	CG	ASN B ASN P	74	4.195	29.223	51.312	1.00	68.17 73.30
	2150	OD1	ASN B	74	3.211	29.829	52.267	1.00	73.30 72.42
	2151	ND2	ASN B	74 74	2.787	29.182	53.225	1.00	62.22
	2152	C	ASN B	74 74	2.831	31.081	52.014	1.00	85.31
60	2153	0	ASN B	74	6.251	27.885	51.066	1.00	73.92
60	2154	N	GLU B	75	7.342 5.612	28.142	50.543	1.00	73.43
	2155	CA	GLU B	75	6.138	26.732	50.891	1.00	82.35
	2156	CB	GLU B	75	5.450	25.682 24.338	50.029	1.00	88.01
	2157	CG	GLU B	75	5.962	24.338 23.548	50.297	1.00	88.41
65	2158	CD	GLU B	75	5.673	23.548 22.053	51.490	1.00	102.21
03	2159	OE1	GLU B	75	4.497	21.692	51.358	1.00	103.43
	2160 2161	OE2	GLU B	75	6.622	21.242	51.118	1.00	95.26
	2162	C	GLU B	75	5.844	26.073	51.493 48.592	1.00	104.69
	2163	0 N	GLU B	75	4.760	26.580	48.592 48.287	1.00	85.00
70	2164	CA	SER B	76	6.799	25.830	47.705	1.00 1.00	92.66
		U A	SER B	76	6.597	26.136	46.299	1.00	74.73
				•					64.93

	2165	CB	SER B	76-	7.811	25.716	45.474	1.00	65.57
	2166	OG.	SER B	76	7.884	24.300	45.366	1.00	53.84
	2167	Ç	SER B	76	5.392	25.350	45.802	1.00	64.12
5	2168	0	SER B	76	4.920	24.425	46.467	1.00	55.19
3	2169	N	GLU B	77	4.891	25.745	44.639	1.00	73.18
	2170	CA	GLU B	77	3.779	25.015	44.046	1.00	69.69
	2171	CB	GLU B	77	3.077	25.874	42.993	1.00	59.63
	2172	CG	GLU B	77	2.498	27.169	43.535	1.00	89.51
10	2173	CD OE1	GLU B	77	1.820	28.000	42.462	1.00	107.00
10	2174 2175	OE2	GLU B GLU B	77	1.798	27.557	41.295	1.00	103.77
	2176	C	GLU B	77 77	1.312	29.093	42.789	1.00	116.96
	2177	ŏ	GLU B	77 77	4.246 5.367	23.698 23.648	43.437	1.00	63.68
	2178	Ň	PRO B	77 78	3.458	23.648 22.659	42.922	1.00	69.58
15	2179	CD	PRO B	78	2.145	22.518	43.542	1.00	56.73
	2180	CA	PRO B	78	3.910	21.387	44.185 42.987	1.00	60.28
	2181	СВ	PRO B	78	2.760	20.438	43.304	1.00 1.00	49.00
	2182	CG	PRO B	78	2.141	21.046	44.534	1.00	42.75
	2183	C	PRO B	78	4.155	21.509	41.497	1.00	68.49 44.78
20	2184	0	PRO B	78	3.483	22.260	40.795	1.00	52.51
	2185	N	VAL B	79	5.137	20.766	41.024	1.00	34.40
	2186	CA	VAL B	79	5.486	20.745	39.616	1.00	23.08
	2187	CB	VAL B	79	6.779	21.527	39.364	1.00	17.91
25	2188	CG1	VAL B	79	7.636	20.834	38.297	1.00	4.69
25	2189	CG2	VAL B	79	6.413	22.948	38.961	1.00	17.83
	2190	C	VAL B	79	5.674	19.278	39.257	1.00	40.76
	2191	0	VAL B	79	6.573	18.609	39.783	1.00	37.75
	2192	N	TYR B	80	4.831	18.773	38.362	1.00	43.38
30	2193	CA	TYR B	80	4.912	17.375	37.992	1.00	37.05
50	2194 2195	CB CG	TYR B TYR B	80	3.510	16.807	37.858	1.00	19.64
	2196	CD1	TYR B	80	2.736	16.988	39.122	1.00	52.81
	2197	CE1	TYR B	80 80	1.881	18.084	39.293	1.00	64.76
	2198	CD2	TYR B	80	1.205 2.901	18.294 16.098	40.505	1.00	83.30
35	2199	CE2	TYR B	80	2.235	16.294	40.186	1.00	64.99
	2200	CZ	TYR B	80	1.390	17.394	41.404 41.559	1.00	80.87
	2201	ОH	TYR B	80	0.754	17.609	42.767	1.00 1.00	84.40
	2202	C	TYR B	80	5.723	17.083	36.752	1.00	76.06 42.78
	2203	0	TYR B	80	5.472	17.622	35.674	1.00	56.71
40	2204	N	LEU B	81	6.716	16.223	36.937	1.00	42.87
	2205	CA	LEV B	81	7.615	15.798	35.878	1.00	47.81
	2206	СВ	LEU B	81	9.049	15.953	36.360	1.00	39.60
	2207	CG	LEU B	81	10.151	15.383	35.481	1.00	53.84
45	2208	CD1	LEU B	81	10.118	16.055	34.119	1.00	61.99
45	2209	CD2	LEU B	81	11.494	15.611	36.160	1.00	65.74
	2210	C	LEU B	81	7.312	14.328	35.562	1.00	60.00
	2211	0	LEU B	81	7.172	13.508	36.467	1.00	72.6
	2212 2213	N CA	GLU B	82	7.208	13.992	34.282	1.00	60.42
50	2214	CB	GLU B GLU B	82	6.888	12.623	33.895	1.00	51.18
30	2215	CG	GLU B	82	5.425	12.559	33.475	1.00	60.43
	2216	CD	GLU B	82 82	4.967 3.453	11.207	32.988	1.00	75.17
	2217	OE1	GLU B	82		11.151	32.824	1.00	92.83
	2218	OE2	GLU B	82	2.880 2.839	12.091 10.166	32.219	1.00	98.53
55	2219	č	GLU B	82	7.778	12.089	33.301	1.00	97.49
	2220	ŏ	GLU B	82	7.734	12.564	32.780 31.645	1.00	49.31
	2221	N	VAL B	83	8.590	11.095	33.116	1.00 1.00	54.46
	2222	CA	VAL B	83	9.512	10.492	32.158	1.00	44.12 51.30
	2223	СВ	VAL B	83	10.656	9.749	32.862	1.00	44.14
60	2224	CG1	VAL B	83	11.654	9.218	31.812	1.00	45.56
	2225	CG2	VAL B	83	11.334	10.669	33.861	1.00	46.11
	2226	Ç	VAL B	83	8.820	9.488	31.246	1.00	55.74
	2227	0	VAL B	83	8.110	8.609	31.713	1.00	73.69
<i>C</i>	2228	N	PHE B	84	9.051	9.608	29.945	1.00	53.23
65	2229	CA	PHE B	84	8.431	8.707	28.981	1.00	49.95
	2230	CB	PHE B	84	7.631	9.481	27.929	1.00	49.58
	2231	CG	PHE B	84	6.436	10.200	28.462	1.00	35.11
	2232	CD1	PHE B	84	6.570	11.175	29.423	1.00	52.71
70	2233	CD2	PHE B	84	5.176	9.913	27.982	1.00	56.24
10	2234	CE1	PHE B	84	5.463	11.859	29.898	1.00	63.67

	2235 2236	CE2 CZ	PHE B	84 ⁻ 84	4.062 4.210	10.595 11.568	28.453 29.414	1.00 1.00	57.29 52.51
	2237	Ç .	PHE B	84	9.495	7.935	28.238	1.00	56.77
5	2238 2239	0 N	PHE B SER B	84	10.696	8.144	28.444	1.00	51.00
,	2240	CA	SER B	85 85	9.021 9.856	7.056 6.236	27.360 26.496	1.00	59.31
	2241	CB	SER B	85	10.382	5.014	27.230	1.00 1.00	53.43
	2242	OG	SER B	85	11.313	4.342	26.403	1.00	52.20 68.06
10	2243	Ç	SER B	85	8.929	5. 79 9	25.372	1.00	61.23
10	2244	0	SER B	85	8.107	4.897	25.547	1.00	56.17
	2245 2246	N CA	ASP B ASP B	86 86	9.053	6.474	24.234	1.00	68.29
	2247	CB	ASP B	86 86	8.228 6.812	6.219 6.736	23.064 23.321	1.00	57.51
	2248	ČG	ASP B	86	5.802	6.181	22.336	1.00 1.00	51.72 90.19
15	2249	OD1	ASP B	86	6.002	6.371	21.113	1.00	100.01
	2250	OD2	ASP B	86	4.811	5.554	22.788	1.00	98.70
	2251 2252	C	ASP B	86	8.868	6.974	21.897	1.00	57.18
	2252 2253	0 N	ASP B TRP B	86 87	9.851 8.330	7.701	22.080	1.00	62.75
20	2254	CA	TRP B	87 87	8.896	6.799 7.483	20.699 19.543	1.00	51.37
	2255	CB	TRP B	87	8.415	6.811	18.264	1.00 1.00	50.71 58.25
	2256	CG	TRP B	87	8.811	5.379	18.134	1.00	53.11
	2257	CD2	TRP B	87	10.032	4.880	17.562	1.00	52.15
25	2258 2259	CE2	TRP B	87	9.945	3.476	17.552	1.00	60.06
25	2259	CE3 CD1	TRP B	87	11.187	5.489	17.054	1.00	60.86
	2261	NE1	TRP B	87 87	8.060 8.734	4.285 3.138	18.452 18.096	1.00	44.63
	2262	CZ2	TRP B	87	10.964	2.672	17.056	1.00 1.00	23.48 78.55
•	2263	CZ3	TRP B	87	12.197	4.691	16.561	1.00	76.55 84.54
30	2264	CH2	TRP B	87	12.077	3.294	16.565	1.00	87.37
	2265	C	TRP B	87	8.545	8.982	19.495	1.00	42.37
	2266 2267	0 N	TRP B LEU B	87 88	9.367 7.308	9.839 9.296	19.123	1.00	23.61
	2268	CA	LEU B	88	6.893	9.296 10.682	19.849 19.837	1.00 1.00	29.09
35	2269	СВ	LEU B	88	5.817	10.944	18.777	1.00	31.21 33.13
	2270	CG	LEU B	88	6.167	10.869	17.290	1.00	18.54
	2271	CD1	LEU B	88	5.021	11.506	16.542	1.00	25.10
	2272 2273	CD2 C	LEV B LEV B	88	7.449	11.594	16.959	1.00	4.59
40	2274	ŏ	LEU B	88 88	6.348 5.517	11.083 10.381	21.182	1.00	40.21
	2275	Ň	LEU B	89	6.815	12.234	21.783 21.644	1.00 1.00	42.92 40.58
	2276	CA	LEU B	89	6.369	12.780	22.912	1.00	31.34
	2277	CB	LEU B	89	7.514	12.805	23.921	1.00	33.17
45	2278 2279	CG	LEU B	89	7.202	13.378	25.299	1.00	42.18
45	2280	CD1 CD2	LEV B	89 89	5.821 8.282	12.933	25.763	1.00	52.47
	2281	C	LEU B	89	5.899	12,923 14,194	26.264 22.621	1.00 1.00	49.06
	2282	ŏ	LEU B	89	6.617	14.973	21.947	1.00	27.75 5.35
50	2283	N	LEU B	90	4.703	14.517	23.109	1.00	4.73
50	2284	CA	LEU B	90	4.149	15.830	22.883	1.00	7.84
	2285 2286	CB CG	LEU B	90	2.634	15.775	22.724	1.00	21.81
	2287	CD1	LEU B	90 90	2.032 2.511	17.148 17.587	22.410 21.026	1.00	21.45
	2288	CD2	LEU B	90	0.521	17.103	21.026 22.464	1.00 1.00	29.29
55	2289	. C	LEU B	90	4.473	16.654	24.087	1.00	15.21 25.07
	2290	0	LEU B	90	3.901	16.441	25.149	1.00	44.25
	2291	N	GLN E	91	5.382	.7.603	23.924	1.00	35.94
	2292 2293	CA CB	GLN B GLN B	91 91	5.768	18.461	25.028	1.00	35.91
60	2294	ÇG	GLN B	91	7.273 8.061	18. 707 1 7.428	24.955 25.129	1.00	17.00
	2295	CD	GLN B	91	9.547	17.637	25.066	1.00 1.00	13.88 35.42
	2296	OE1	GLN B	91	10.092	18.074	24.040	1.00	18.59
	2297	NE2	GLN B	91	10.226	17.318	26.165	1.00	42.81
65	2298 2299	C O	GLN B GLN B	91 01	4.995	19.781	25.025	1.00	36.56
	2300	Ň	ALA B	91 92	4.606 4.761	20.285 20.335	23.966	1.00	49.74
	2301	ČA	ALA B	92	4.054	21.607	26.212 26.313	1.00 1.00	35.59 43.59
	2302	CB	ALA B	92	2.628	21.377	26.734	1.00	43.59 28.50
70	2303	C	ALA B	92	4.719	22.580	27.283	1.00	53.87
70	2304	0	ALA B	92	5.250	22,184	28.318	1.00	69,37

	2305 2306 2307	N CA CB	SER B SER B SER B	93 [.] 93 93	4.684 5.252 4.947	23.860 24.923 26.287	26.932 27.761	1.00 1.00	68.52 64.18
5	2308 2309 2310	OG C O	SER B SER B SER B	93 93 93	3.537 4.593 5.200	26.475 26.475 24.849 25.163	27.133 26.986 29.128	1.00 1.00 1.00	72.74 77.53 56.86
	2311 2312 2313	N CA CB	ALA B ALA B	94 94	3.336 2.560	24.430 24.304	30.143 29.131 30.346	1.00 1.00 1.00	67.19 36.84 46.61
10	2314 2315	CO	ALA B ALA B	94 94 94	2.296 1.248 0.553	25.671 23.611 24.008	30.923 29.999 29.063	1.00 1.00 1.00	39.28 57.58 64.68
15	2316 2317 2318	N CA CB	GLU B GLU B GLU B	95 95 95	0.912 -0.311 -0.290	22.571 21.824 20.535	30.754 30.510 31.329	1.00 1.00 1.00	65.01 66.91 69.50
13	2319 2320 2321	CG CD OE1	GLU B GLU B GLU B	95 95 95	0.872 0.886 1.716	19.619 18.326 17.452	30.950 31.738 31.415	1.00 1.00 1.00	64.00 82.38 86.38
20	2322 2323 2324	OE2 C O	GLU B GLU B GLU B	95 95 95	0.075 -1.540 -2.644	18.181 22.669 22.394	32.678 30.831 30.346	1.00 1.00 1.00	93.94 68.95 67.01
	2325 2326 2327	N CA CB	VAL B VAL B VAL B	96 96 96	-1.345 -2.442 -3.012	23.703 24.603 24.282	31.644 31.996 33.374	1.00 1.00 1.00	72.58 72.17 56.87
25	2328 2329 2330	CG1 CG2 C	VAL B VAL B VAL B	96 96 96	-4.277 -3.280 -1.980	25.079 22.788 26.059	33.592 33.489 31.988	1.00 1.00 1.00	54.83 38.14 76.73
20	2331 2332 2333	O N CA	VAL B VAL B VAL B	96 97 97	-1.079 -2.611 -2.258	26.441 26.867 28.271	32.738 31.141 30.996	1.00 1.00 1.00	76.80 80.52 82.56
30	2334 2335 2336	CB CG1 CG2	VAL B VAL B VAL B	97 97 97	-1.740 -1.543 -0.429	28.546 30.029 27.803	29.562 29.341 29.334	1.00 1.00 1.00	85.79 102.89 95.31
35	2337 2338 2339	C O N	VAL B VAL B MET B	97 97 98	-3.420 -4.591 -3.073	29.216 28.885 30.394	31.283 31.041 31.807	1.00 1.00 1.00	82.63 75.81 84.13
	2340 2341 2342	CA CB CG	MET B MET B MET B	98 98 98	-4.050 -3.430 -3.324	31.442 32.509 32.120	32.112 33.020 34.480	1.00 1.00 1.00	91.67 102.42
40	2343 2344 2345	SD CE C	MET B MET B MET B	98 98 98	-4.951 -5.607 -4.488	31.748 33.383 32.107	35.181 35.438 30.808	1.00 1.00	120.32 137.79 124.64
	2346 2347 2348	O N CA	MET B GLU B GLU B	98 99 99	-3.637 -5.797 -6.266	32.555 32.193 32.803	30.027 30.571	1.00 1.00 1.00	86.05 83.23 75.14
45	2349 2350 2351	CB CG CD	GLU B GLU B GLU B	99 99 99	-7.745 -8.228 -9.693	33.156 33.862	29.334 29.408 28.144	1.00 1.00 1.00	80.10 83.15 109.03
50	2352 2353 2354	OE1 OE2 C	GLU B GLU B	99 99 99	-10.084 -10.446	34.250 34.917 33.893	28.204 29.189 27.265	1.00 1.00 1.00	121.43 131.12 120.08
	2355 2356 2357	O N CA	GLU B GLY B	કડ 100	-5.477 -5.371 -4.915	34.059 34.955 34.113	29.019 29.846 27.818	1.00 1.00 1.00	76.85 76.94 81.06
55	2358 2359 2360	C O N	GLY B GLY B GLY B GLN B	100 100 100	-4.139 -2.644 -1.877	35.273 35.015 35.674	27.429 27.460 26.752	1.00 1.00 1.00	80.78 77.00 79.67
	2361 2362 2363	CA CB CG	GLN B GLN B GLN B	101 101 101	-2.220 -0.798 -0.494	34.062 33.729 32.996	28.284 28.370 29.682	1.00 1.00 1.00	75.05 78.99 84.76
60	2364 2365 2366	CD OE1 NE2	GLN B	101 101 101	-0.561 0.340 -0.007	33.870 35.097 36.083	30.924 30.817 30.156	1.00 1.00 1.00	92.38 98.22 100.31
65	2367 2368 2369	CO	GLN B GLN B GLN B	101 101 101	1.509 -0.351 -1.169	35.036 32.876 32.375	31.456 27.178 26.414	1.00 1.00 1.00	92.08 65.25 57.39
03	2370 2371	N CD CA	PRO B PRO B PRO B	102 102 102	0.963 2.093 1.422	32.708 33.382 31.901	26.997 27.653 25.868	1.00 1.00 1.00	59.88 62.83 59.94
70	2372 2373 2374	CB CG C	PRO B PRO B PRO B	102 102 102	2.864 3.284 1.313	32.365 32.645 30.411	25.683 27.070 26.120	1.00 1.00 1.00	48.67 63.93 60.51

	2375 2376	0 N	PRO B LEU B	102 103	1.559	29.938	27.220	1.00	71.07
	2377	ČA	LEU B	103	0.926 0.780	29.686 28.238	25.081 25.119	1.00	66.31
_	2378	CB	LEU B	103	-0.664	27.880	24.821	1.00 1.00	56.78 50.78
5	2379	CG	LEU B	103	-0.974	26.402	24.666	1.00	77.35
	2380	CD1	LEU B	103	-0.629	25.680	25.955	1.00	76.88
	2381	CD2	LEU B	103	-2.450	26.229	24.318	1.00	77.48
	2382	C	LEU B	103	1.703	27.688	24.030	1.00	54.03
10	2383 2384	O N	LEU B PHE B	103	1.554	28.025	22.857	1.00	55.72
10	2385	ČA	PHE B	104 104	2.655 3.607	26.842 26.332	24.402	1.00	48.78
	2386	CB	PHE B	104	4.979	26.893	23.414 23.748	1.00	45.32
	2387	ÇG	PHE B	104	5.976	26.705	23.746 22.677	1.00 1.00	32.16 32.32
	2388	CD1	PHE B	104	6.158	27.689	21.717	1.00	39.73
15	2389	CD2	PHE B	104	6.770	25.566	22.641	1.00	39.96
	2390	CE1	PHE B	104	7.123	27.544	20.708	1.00	55.96
	2391	CE2	PHE B	104	7.744	25.404	21.638	1.00	63.91
	2392	cz	PHE B	104	7.923	26.404	20.673	1.00	61.86
20	2393 2394	C O	PHE B PHE B	104	3.700	24.805	23.299	1.00	42.46
20	2395	N	LEU B	104 105	4.206 3.223	24.140 24.250	24.199	1.00	46.85
	2396	CA	LEU B	105	3.223	24.250 22.811	22.190 22.006	1.00	35.08
	2397	CB	LEU B	105	1.999	22.311	21.356	1.00 1.00	22.82 37.29
	2398	CG	LEU B	105	0.804	22.355	22.298	1.00	42.12
25	2399	CD1	LEU B	105	-0.404	21.635	21.660	1.00	56.32
	2400	CD2	LEU B	105	1.196	21.673	23.579	1.00	54.72
	2401	Ç	LEU B	105	4.468	22.421	21.165	1.00	23.23
	2402	0	LEU B	105	5.055	23.250	20.476	1.00	30.46
30	2403	N	ARG B	106	4.833	21.149	21.226	1.00	15.51
30	2404 2405	CA CB	ARG B	106	5.990	20.674	20.475	1.00	30.48
	2406	CG	ARG B ARG B	106	7.249	21.056 20.446	. 21.243	1.00	25.17
	2407	CD	ARG B	106 106	8.540 9.631	20. 446 20.546	20.746	1.00	50.57
	2408	NE	ARG B	106	10.970	20.223	21.842 21.346	1.00 1.00	51.15 50.88
35	2409	CZ	ARG B	106	12.013	19.938	22.120	1.00	42.48
	2410	NH1	ARG B	106	11.875	19.937	23.436	1.00	52.91
	2411	NH2	ARG B	106	13.191	19.650	21.581	1.00	40.82
	2412	C	ARG B	106	5.913	19.143	20.289	1.00	37.36
40	2413	0	ARG B	106	5.488	18.406	21.199	1.00	26.46
40	2414	N	CYS B	107	6.304	18.660	19.113	1.00	28.15
	2415 2416	CA C	CYS B CYS B	107	6.250	17.231	18.860	1.00	29.34
	2417	ŏ	CYS B	107 107	7.669 8.280	16.735 16.584	18.872	1.00	42.87
	2418	СВ	CYS B	107	5.617	16.945	17.812 17.502	1.00	35.58
45	2419	SG	CYS B	107	5.072	15.220	17.305	1.00 1.00	38.81 55.53
	2420	N	HIS B	108	8.173	16.481	20.081	1.00	42.37
	2421	CA	HIS B	108	9.544	16.022	20.296	1.00	43.07
	2422	СВ	HIS B	108	9.947	16.267	21.751	1.00	59.40
50	2423	CG	HIS B	108	11.374	15.931	22.052	1.00	55.40
30	2424 2425	CD2	HIS B	108	11.925	15.232	23.068	1.00	55.98
	2426	ND1 CE1	HIS B HIS B	108	12.421	16.349	21.259	1.00	54.99
	2427	NE2	HIS B	108 108	13.558 13.286	15.919	21.776	1.00	62.39
	2428	C	HIS B	108	9.739	15.239 14.563	22.874 19.946	1.00	62.88
55	2429	ŏ	HIS B	108	9.008	13.698	20.440	1.00 1.00	36.76 16.46
	2430	N	GLY B	109	10.733	14.307	19.097	1.00	27.59
	2431	CA	GLY B	109	11.001	12.953	18.656	1.00	39.81
	2432	C	GLY B	109	12.066	12.233	19.446	1.00	36.02
60	2433	0	GLY B	109	13.025	12.841	19.903	1.00	45.53
60	2434	N	TRP B	110	11.902	10.925	19.589	1.00	45.09
	2435 2436	CA	TRP B	110	12.842	10.094	20.328	1.00	42.50
	2437	CB CG	TRP B	110	12.456	8.614	20.147	1.00	42.85
	2438	CD2	TRP B	110 110	13.388 13,360	7. 7 39 7.449	20.893	1.00	47.55 54.49
65	2439	CE2	TRP B	110	14.455	6.601	22.295 22.586	1.00 1.00	54.18 43.50
	2440	CE3	TRP B	110	12.518	7.855	23.339	1.00	57.45
	2441	CD1	TRP B	110	14.459	7.056	20.399	1.00	57.45 51.38
	2442	NE1	TRP B	110	15.108	6.357	21.409	1.00	48.13
70	2443	CZ2	TRP B	110	14.729	6.151	23.872	1.00	33.15
70	2444	CZ3	TRP B	110	12.793	7.403	24.629	1.00	55.46

	2445 2446	CH2 C	TRP B	110 110	13.894 14.276	6.557 10.354	24.877 19.886	1.00	49.35
	2447	ŏ.	TRP B	110	14.544	10.511	18.690	1.00 1.00	45.65
	2448	Ň	ARG B	111	15.182	10.388	20.866	1.00	34.73
5	2449	CA	ARG B	111	16.604	10.644	20.631	1.00	55.00 60.99
	2450	CB	ARG B	111	17.254	9.438	19.949	1.00	56.42
	2451°	CG	ARG B	111	17.586	8.319	20.926	1.00	78.50
	2452	CD	ARG B	111	18.140	7.100	20.224	1.00	104.44
10	2453	NE	ARG B	111	18.757	6.157	21.154	1.00	117.08
10	2454	CZ	ARG B	111	19.996	6.272	21.628	1.00	124.78
	2455	NH1	ARG B	111	20.766	7.291	21.261	1.00	125.05
	2456 2457	NH2	ARG B	111	20.463	5.363	22.473	1.00	126.10
	2457	C	ARG B ARG B	111 111	16.813	11.896	19.790	1.00	67.62
15	2459	Ň	ASN B	112	17.751 15.934	11.974 12.876	19.000	1.00	74.03
	2460	CA	ASN B	112	16.039	14.116	19.978 19.228	1.00	69.44
	2461	CB	ASN B	112	17.207	14.964	19.725	1.00 1.00	76.51 84.90
	2462	CG	ASN B	112	17.150	16.373	19.160	1.00	106.45
	2463	OD1	ASN B	112	16.253	16.734	18.385	1.00	105.76
20	2464	ND2	ASN B	112	18.134	17.183	19.546	1.00	117.72
	2465	C	ASN B	112	16.155	13.785	17.751	1.00	79.76
	2466	0	ASN B	112	16.695	14.568	16.973	1.00	88.06
	2467 2468	N	TRP B	113	15.686	12.614	17.372	1.00	76.72
25	2469	CA CB	TRP 8	113	15.721	12.245	15.953	1.00	59. 9 5
23	2470	CG	TRP B	113 113	15.222 16.236	10.811	15.765	1.00	54.79
	2471	CD2	TRP B	113	16.236	9.821 8.442	16,180	1.00	40.29
	2472	CE2	TRP B	113	17.312	7.914	16.523 16.846	1.00 1.00	18.18
	2473	CE3	TRP B	113	14.930	7.603	16.587	1.00	22.19
30	2474	CD1	TRP B	113	17.574	10.060	16.308	1.00	12.77 42.86
	2475	NE1	TRP B	113	18.226	8.922	16.707	1.00	25.08
	2476	CZ2	TRP B	113	17.493	6.587	17.228	1.00	22.94
	2477	CZ3	TRP B	113	15.111	6.286	16.966	1.00	28.48
35	2478	CH2	TRP B	113	16.383	5.790	17.281	1.00	24.73
55	2479 2480	C O	TRP B	113	14.836	13.224	15.194	1.00	65.32
	2481	Ň	TRP B ASP B	113 114	13.936	13.822	15.777	1.00	68.76
	2482	ČA	ASP B	114	15.057 14.164	13.403 14.252	13.912	1.00	50.94
	2483	CB	ASP B	114	14.767	14.536	13.145 11.768	1.00 1.00	52.0 9
40	2484	CG	ASP B	114	16.039	15.346	11.830	1.00	52.20 66.27
	2485	OD1	ASP B	114	16.065	16.368	12.546	1.00	80.90
	2486	OD2	ASP B	114	17.011	14.967	11.147	1.00	65.81
	2487	Ç	ASP B	114	12.798	13.615	13.004	1.00	54.32
45	2488	0	ASP B	114	12.676	12.397	13.005	1.00	49.44
43	2489 2490	N CA	VAL B	115	11.762	14.429	12.886	1.00	59.6 5
	2490	CA CB	VAL B VAL B	115	10.408	13.936	12.713	1.00	44.63
	2492	CG1	VAL B	115 115	9.542 8.162	14.291 13.697	13.899	1.00	43.22
	2493	CG2	YAL B	115	10.192	13.802	13.715 15.156	1.00 1.00	33.45
50	2494	C	VAL B	115	9.876	14.672	11.497	1.00	33.33 60.55
	2495	0	VAL B	115	10.254	15.827	11.261	1.00	71.83
	2496	N	TYR B	116	9.023	14.021	10.715	1.00	48.40
	2497	CA	TYR B	116	8.490	14.684	9.543	1.00	29.55
55	2498	СВ	TYR B	116	9.214	14.204	8.299	1.00	25.24
22	2499 2500	CG	TYR B	116	10.708	14.436	8.299	1.00	28.14
	2501	CD1 CE1	TYR B	116	11.582	13.475	8.783	1.00	40.15
	2502	CD2	TYR B TYR B	116 116	12.956 11.250	13.645	8.691	1.00	52.64
	2503	CE2	TYR B	116	12.635	15.590 15.770	7.745	1.00	41.11
60	2504	CZ	TYR B	116	13.478	14.797	7.651 8.127	1.00 1.00	48.69 44.88
	2505	ОН	TYR B	116	14.841	14.957	8.017	1.00	54.67
	2506	С	TYR B	116	6.991	14.501	9.377	1.00	27.78
	2507	0	TYR B	116	6.383	13.681	10.051	1.00	28.35
65	2508	N	LYS B	117	6.409	15.265	8.460	1.00	38.88
U.)	2509	CA	LYS B	117	4.976	15.213	8.227	1.00	37.83
	2510 2511	CB	LYS B	117	4.567	13.922	7.508	1.00	47.24
	2512	CG CD	LYS B Lys b	117	4.732	13.956	5.998	1.00	69.83
	2513	CE	LYS B	117 117	4.053 2.549	12.743 12.718	5.350	1.00	93.57
70	2514	NZ	LYS B	117	1.865	12.716 11.498	5.644 5.113	1.00	101.93
-		· · -		• • • •	1.505	11.730	5.113	1.00	91.83

	2515 2516	CO	LYS B	117 117	4.347 3.695	15.264 14.319	9.603 10.041	1.00 1.00	25.37 28.98
	2517 2518	N CA	VAL B VAL B	118 118	4.568	16.374	10.296	1.00	23.24
5	2519	CB	VAL B	118	4.014 4.919	16.513 17.367	11.629 12.545	1.00 1.00	23.69
	2520	CG1	VAL B	118	4.205	17.627	13.868	1.00	38.59 45.19
	2521 2522	CG2 C	VAL B VAL B	118 118	6.254 2.650	16.648	12.795	1.00	18.15
	2523	ŏ	VAL B	118	2.462	17.152 18.227	11.593 11.006	1.00 1.00	18.84
10	2524	N	ILE B	119	1.700	16.503	12.250	1.00	8.55 12.98
	2525 2526	CA CB	ILE B	119 119	0.355	17.026	12.293	1.00	30.22
	2527	CG2	ILE B	119	-0.627 -2.064	16.130 16.621	11.498 11.688	1.00 1.00	46.31
1.5	2528	CG1	ILE B	119	-0.236	16.112	10.019	1.00	42.76 21.93
15	2529 2530	CD1 C	ILE B	119	-1.236	15.436	9.133	1.00	51.60
	2531	ŏ	ILE B	119 119	-0.076 0.261	17.038 16.123	13.734 14.483	1.00 1.00	38.62
	2532	N	TYR B	120	-0.818	18.068	14.125	1.00	47.55 32.69
20	2533 2534	CA CB	TYR B TYR B	120	-1.312	18.148	15.489	1.00	32.47
20	2535	CG	TYR B	120 120	-0.950 0.503	19.474 19.596	16.123 16.455	1.00	16.42
	2536	CD1	TYR B	120	1.419	20.056	15.515	1.00 1.00	25.56 35.91
	2537 2538	CE1	TYR B	120	2.771	20.205	15.844	1.00	51.47
25	2539	CD2 CE2	TYR B TYR B	120 120	0.966 2.311	19.275	17.728	1.00	32.05
	2540	CZ	TYR B	120	3.209	19,412 19.883	18.070 17.123	1.00 1.00	29.56 44.13
	2541	ОН	TYR B	120	4.537	20.063	17.438	1.00	29.40
	2542 2543	C	TYR B TYR B	120	-2.806	18.001	15.490	1.00	33.00
30	2544	Ň	TYR B	120 121	-3.484 -3.322	18.535 17.277	14.625 16.467	1.00	54.53
	2545	CA	TYR B	121	-4.744	17.066	16.544	1.00 1.00	31.54 38.10
	2546 2547	CB	TYR B	121	-5.068	15.570	16.402	1.00	34.72
	2547 2548	CG CD1	TYR B TYR B	121 121	-4.635 -3.293	14.953 14.656	15.087	1.00	45.90
35	2549	CE1	TYR B	121	-2.878	14.083	14.855 13.654	1.00 1.00	43.35 44.63
	2550	CD2	TYR B	121	-5.570	14.659	14.076	1.00	45.04
	2551 2552	CE2 CZ	TYR B TYR B	121 121	-5.169 -3.822	14.078	12.874	1.00	37.76
	2553	OH	TYR B	121	-3.622 -3.411	13.796 13.225	12.675 11.502	1.00 1.00	47.75 43.41
40	2554	C	TYR B	121	-5.272	17.579	17.864	1.00	51.86
	2555 2556	0 N	TYR B LYS B	121 122	-4.735	17.246	18.927	1.00	65.44
	2557	CA	LYS B	122	-6.314 -6.957	18.403 18.914	17.794 18.992	1.00 1.00	51.19
45	2558	CB	LYS B	122	-7.037	20.435	18.969	1.00	60.52 58.03
45	2559 2560	CG CD	LYS B	122	-7.268	21.024	20.357	1.00	76.69
	2561	CE	LYS B LYS B	122 122	-7.727 -9.203	22.472 22.561	20.312 19.973	1.00	76.94
	2562	NZ	LYS B	122	-9.694	23.961	20.057	1.00 1.00	78.85 78.17
50	2563	C	LYS B	122	-8.368	18.331	19.016	1.00	69.22
30	2564 2565	0 N	LYS B ASP B	122 123	-9.259	18.817	18.314	1.00	71.75
	2566	CA	ASP B	123	-8.554 -9.840	17.283 16.611	19.814 19.936	1.00 1.00	75.25 81.83
	2567	CB	ASP B	123	-10.952	17.623	20.242	1.00	85.33
55	2568 2569	CG OD1	ASP B	123	-10.809	18.253	21.618	1.00	86.97
<i>55</i>	2570	OD2	ASP B ASP B	123 123	-10.750 -10.764	17.499 19.501	22.613 21.703	1.00	97.59
	2571	С	ASP B	:23	-10.172	15.841	18.660	1.00 1.00	80.57 85.87
	2572	0	ASP B	123	-11.183	16.107	18.002	1.00	90.87
60	2573 2574	N CA	GLY B GLY B	124 124	-9.310 -9.538	14.889	18.314	1.00	83.44
	2575	Č.	GLY B	124	-9.383	14.080 14.835	17.131 15.826	1.00 1.00	83.47 82.06
	2576	0	GLY B	124	-9.053	14.236	14.804	1.00	80.62
	2577 2578	N CA	GLU B	125	-9.615	16.144	15.847	1.00	76.60
65	2579	CB	GLU B GLU B	125 125	-9.479 -10.431	16.951 18.146	14.640 14.697	1.00	69.95
	2580	CG	GLU B	125	-11.903	17.778	14.854	1.00 1.00	83.15 99.12
	2581	CD CD	GLU B	125	-12.808	19.009	14.961	1.00	110.18
	2582 2583	OE1 OE2	GLU B GLU B	125 125	-12.287 -14.041	20.153 18.828	14.909	1.00	115.12
70	2584	c_	GLU B	125	-8.043	17.452	15.099 14.501	1.00 1.00	112.68 59.20
							,		

	2585	0	GLU B	125	-7.370	17.681	15.493	1.00	
	2586	N	ALA B	126	-7.574	17.609	13.269	1.00 1.00	68.90 55.84
	2587 2588	CA CB	ALA B ALA B	126	-6.221	18.112	13.032	1.00	49.26
5	2589	C	ALA B	126 126	-5.783 -6.229	17.788 19.623	11.636	1.00	37.55
	2590	Õ	ALA B	126	-7.288	20.251	13.229 13.192	1.00 1.00	55.35
	2591	N	LEU B	127	-5.053	20.211	13.425	1.00	62.37 58.36
	2592 2593	CA CB	LEU B LEU B	127	-4.968	21.648	13.652	1.00	56.69
10	2594	CG	LEU B	127 127	-4.821 -4.606	21.938 23.411	15.148 15.496	1.00	64.48
	2595	CD1	LEU B	127	-5.705	24.262	14.864	1.00 1.00	71.37 76.49
	2596	CD2	LEU B	127	-4.590	23.573	17.012	1.00	74.87
	2597 2598	C	LEU B LEU B	127 127	-3.837	22.314	12.895	1.00	59.25
15	2599	Ň	LYS B	128	-3.979 -2.710	23.463 21.619	12.449 12.760	1.00 1.00	65,52
	2600	CA	LYS B	128	-1.583	22.176	12.022	1.00	39.64 49.21
	2601 2602	CB CG	LYS B LYS B	128	-0.695	23.067	12.911	1.00	55.50
	2603	CD	LYS B	128 128	-1.370 -0.363	24.362 25.479	13.365	1.00	77.67
20	2604	CE	LYS B	128	-1.085	26.778	13.615 13.981	1.00 1.00	85.20 95.26
	2605	NZ	LYS B	128	-0.159	27.945	14.093	1.00	94.69
	2606 2607	CO	LYS B Lys b	128 128	-0.743	21.091	11.397	1.00	47.41
	2608	Ň	TYR B	129	-0.639 -0.181	19.967 21.412	11.917 10.277	1.00 1.00	56.27
25	2609	CA	TYR B	129	0.682	20.491	9.551	1.00	25.40 31.17
	2610	CB	TYR B	129	-0.094	19.800	8.429	1.00	9.94
	2611 2612	CG CD1	TYR B TYR B	129 129	0.773	. 18.963	7.516	1.00	7.68
	2613	CE1	TYR B	129	0.995 1.788	17.618 16.850	7.780 6. 94 8	1.00 1.00	13.54
30	2614	CD2	TYR B	129	1.370	19.519	6.393	1.00	15.62 9.74
	2615 2616	CE2 CZ	TYR B	129	2.164	18.759	5.558	1.00	6.56
	2617	OH	TYR B TYR B	129 129	2.369 3.160	17.425 16.667	5.839	1.00	23.46
25	2618	C	TYR B	129	1.905	21,203	5.007 8.987	1.00 1.00	29.69 18.84
35	2619	0	TYR B	129	1.810	22.418	8.723	1.00	20.48
	2620 2621	N CA	TRP B	130 130	2.983	20.508	8.856	1.00	10.01
	2622	CB	TRP B	130	4.195 4.621	21.121 22.248	8.376 9.331	1.00 1.00	26.80
40	2623	CG	TRP B	130	5.657	23.141	8.763	1.00	24.97 34.86
40	2624 2625	CD2 CE2	TRP B	130	5.463	24.474	8.258	1.00	19.75
	2626	CE3	TRP B TRP B	130 130	6.718 4.338	24.933 25.321	7.789	1.00	18.96
	2627	CD1	TRP B	130	6.995	22.854	8.160 8.577	1.00 1.00	4.59 46.79
45	2628	NE1	TRP B	130	7.637	23.935	7.990	1.00	33.27
47	2629 2630	CZ2 CZ3	TRP B TRP B	130 130	6.887 4.513	26.195	7.230	1.00	7.20
	2631	CH2	TSP B	130	5.778	26.582 27.003	7.599 7.141	1.00 1.00	26.73
	2632	C	TRP B	130	5.204	19.990	8.359	1.00	33.91 28.67
50	2633 2634	0 N	TRP B	130	5.511	19.385	9.388	1.00	37.85
50	2635	CA	TYR B TYR B	131 131	5.686 6.639	19.697 18.631	7.164	1.00	25.88
	2636	CB	TYR B	131	7.327	18.864	6.919 5.599	1.00 1.00	25.53 12.69
	2637	CG	TYR B	131	8.003	17.638	5.076	1.00	27.25
55	2638 2639	CD1 CE1	TYR B TYR B	131 131	7.258	16.534	4.672	1.00	27.89
	2640	CD2	TYR B	131	7.893 9.385	15.406 17.589	4.143 4. 94 9	1.00 1.00	37.49
	2641	CE2	TYR B	131	10.030	16.477	4.424	1.00	47.62 47.79
	2642 2643	CZ	TYR B	131	9.287	15.394	4.023	1.00	46.72
60	2644	OH C	TYR B TYR B	131 131	9.948 7.699	14.315	3.487	1.00	44.87
	2645	ŏ	TYR B	131	7.730	18.490 17.491	7.988 8.714	1.00 1.00	41.53 45.44
	2646	N	GLU B	132	8.584	19.481	8.058	1.00	41.35
	2647 2648	CA CB	GLU B	132	9.651	19.477	9.045	1.00	23.47
65	2649	ca	GLU B	132 132	10.631 11.512	20.595 20.343	8.746 7.517	1.00	26.69
	2650	CD	GLU B	132	12.674	19.419	7.517 7.819	1.00 1.00	30.91 59.01
	2651 2652	OE1	GLU B	132	12.695	18.835	8.933	1.00	78.14
	2652 2653	OE2 C	GLU B	132 132	13.555	19.276	6.939	1.00	45.30
70	2654	ŏ	GLU B	132	9.017 7.926	19.678 20.252	10.410 10.503	1.00 1.00	30.80 15.18
									10.10

	2655 2656	N CA	ASN B	133 133	9.673 9.078	19.198 19.340	11.466 12.785	1.00 1.00	38.68 35.69
	2657 2658	CB:	ASN B	133	9.969	18.765	13.884	1.00	24.76
5 ,	2659	CG . OD1	ASN B ASN B	133 133	9.165	18.350	15.126	1.00	52.21
٠,	2660	ND2	ASN B	133	8.183 9.582	19.018 17.243	15.524	1.00	35.03
	2661	C	ASN B	133	9.562 8.857	20.813	15.745	1.00	43.95
	2662	ŏ	ASN B	133	9.651	21.644	13.030 12.587	1.00 1.00	29.20
	2663	N	HIS B	134	7.770	21.132	13.718	1.00	43.35
10	2664	CA	HIS B	134	7.435	22.506	14.022	1.00	15.66 21.19
	2665	CB	HIS B	134	6.522	23.054	12.927	1.00	41.57
	2666	CG	HIS B	134	5.268	22.256	12.734	1.00	45.84
	2667	CD2	HIS B	134	3.972	22.543	12.990	1.00	30.22
15	2668 2669	ND1 CE1	HIS B	134	5.280	20.969	12.228	1.00	29.02
13	2670	NE2	HIS B HIS B	134 134	4.037 3.230	20.507 21.443	12.183	1.00	45.78
	2671	C	HIS B	134	6.733	21. 44 3 22.587	12.640	1.00	39.55
	2672	ŏ	HIS B	134	6.072	21.631	15.380 15.826	1.00 1.00	30.10
	2673	N	ASN B	135	6.871	23.731	16.043	1.00	22.57 35.59
20	2674	CA	ASN B	135	6.263	23.933	17.355	1.00	43.05
	2675	CB	ASN B	135	7.182	24.741	18.303	1.00	49.56
	2676	CG	ASN B	135	8.585	24.138	18.481	1.00	62.83
	2677	OD1	ASN B	135	8.717	22.936	18.749	1.00	59.97
25	2678 2679	ND2 C	ASN B ASN B	135	9.614	24.991	18.356	1.00	50.35
20	2680	ŏ	ASN B	135 135	5.006 5.024	24.761	17.162	1.00	31.65
	2681	Ň	ILE B	136	3.910	25.700 24.406	16.384	1.00	53.46
	2682	CA	ILE B	136	2./20	25.244	17.820 17.749	1.00 1.00	39.40
	2683	CB	ILE B	136	1.440	24.484	18.081	1.00	46.75 51.16
30	2684	CG2	ILE B	136	0.254	25.448	18.105	1.00	27.02
	2685	CG1	ILE B	136	1.232	23.368	17.065	1.00	48.68
	2686	CD1	ILE B	136	-0.057	22.599	17.259	1.00	57.62
	2687 2688	C	ILE B	136	2.922	26.304	18.834	1.00	57.38
35	2689	0 N	ILE B SER B	136	2.996	25.995	20.026	1.00	38.50
55	2690	CA	SER B	137 137	3.035 3.238	27.554 28.653	18.409	1.00	62.66
	2691	CB	SER B	137	4.495	29.443	19.333 18.941	1.00 1.00	62.59
	2692	OG	SER B	137	4.789	30.448	19.899	1.00	62.06 70.77
40	2693	C	SER B	137	2.015	29.557	19.314	1.00	54.31
40	2694	0	SER B	137	1.675	30.140	18.295	1.00	61.87
	2695	N	ILE B	138	1.344	29.665	20.450	1.00	57.19
	2696 2697	CA CB	ILE B	138	0.167	30.511	20.551	1.00	64.51
	2698	CG2	ILE B	138 138	-1.060	29.702	20.970	1.00	66.59
45	2699	CG1	ILE B	138	-2.289 -1.244	30.588 28.528	20.965	1.00	62.45
	2700	CD1	ILE B	138	-2.439	27.657	20.011 20.338	1.00 1.00	72.23
	2701	C	ILE 5	138	0.409	31.600	21.581	1.00	72.19 70.00
	2702	0	ILE B	138	0.207	31.396	22.777	1.00	80.22
50	2703	N	THR B	139	0.846	32.760	21.100	1.00	75.14
50	2704	CA	THR B	139	1.143	33.914	21.951	1.00	76.04
	2705 2706	CB	THR B	139	1.419	35.149	21.086	1.00	66.84
	2707	OG1 CG2	THR B THR B	139	0.347	35.322	20.153	1.00	70.10
	2708	C	THR B	139 139	2.720 0.064	34.969 34.246	20.312	1.00	62,07
55	2709	ŏ	THR B	139	0.333	34.206	22.993 24.190	1.00 1.00	77.29
	2710	N	ASN B	140	-1.142	34.598	22.553	1.00	88. 7 8 78.71
	2711	CA	ASN B	140	-2.244	34.893	23.485	1.00	86.24
	2712	CB	ASN B	140	-2.994	36.169	23.082	1.00	96.34
60	2713	CG	ASN B	140	-2.195	37.465	23.304	1.00	113.86
00	2714 2715	OD1	ASN B	140	-2.591	38.486	22.747	1.00	123.78
	2716	ND2	ASN B	140	-1.120	37.473	24.100	1.00	121.56
	2717	C	ASN B ASN B	140	-3.245	33.716	23.456	1.00	84.41
	2718	Ň	ALA B	140 141	-3.962 -3.298	33.521 32.944	22.474	1.00	92.35
65	2719	CA	ALA B	141	~3.296 -4.186	32. 944 31.781	24.536 24.642	1.00	74.85
	2720	СВ	ALA B	141	-3.768	30.931	24.642 25.819	1.00 1.00	70.00 60.72
	2721	С	ALA B	141	-5.879	32.080	24.744	1.00	73.54
	2722	0	ALA B	141	-6.083	33.215	25.000	1.00	71.12
70	2723	N	THR B	142	-6.486	31.033	24.557	1.00	79.19
70	2724	CA	THR B	142	-7.945	31.135	24.602	1.00	81.65

	2725	CB	THR B	142	-8.550	31.294	23.191	1.00	07.55
	2726	OG1	THR B	142	-7.856	32.324	22.475	1.00	87.55 87.31
	2727	CG2	THR B	142	-10.032	31.647	23.292	1.00	80.50
5	2728	C	THR B	142	-8.556	29.872	25.196	1.00	81.42
3	2729 2730	O N	THR B	142	-8.001	28.782	25.063	1.00	80.47
	2730 2731	CA	VAL B VAL B	143	-9.716	30.022	25.828	1.00	79.19
	2732	CB	VAL B	143 143	-10.385 -11.681	28.881	26.436	1.00	80.64
	2733	CG1	VAL B	143	-12.667	29.314 29.899	27.154	1.00	85.23
10	2734	CG2	VAL B	143	-12.293	28.123	26.146 27.880	1.00 1.00	91.61
	2735	С	VAL B	143	-10.728	27.848	25.370	1.00	91.42
	2736	0	VAL B	143	-10.878	26.659	25.659	1.00	78.44 67.92
	2737	N	GLU B	144	-10.847	28.317	24.132	1.00	87.88
15	2738	CA	GLU B	144	-11.173	27.438	23.019	1.00	94.42
13	2739 2740	CB	GLU B	144	-11.546	28.261	21.775	1.00	103.89
	2740 2741	CG CD	GLU B GLU B	144	-12.116	27.439	20.605	1.00	127.47
	2742	OE1	GLU B	144 144	-13.460	26.781	20.925	1.00	145.47
	2743	OE2	GLU B	144	-14.018 -13.960	27.052 25.995	22.011	1.00	154.66
20	2744	C	GLU B	144	-9.977	26.546	20.087 22.721	1.00 1.00	153.18
	2745	0	GLU B	144	-10.137	25.385	22.328	1.00	87.49 92.98
	2746	N	ASP B	145	-8.777	27.086	22.919	1.00	73.99
	2747	CA	ASP B	145	-7.557	26.336	22.674	1.00	73.40
25	2748	CB	ASP B	145	-6.348	27.253	22.815	1.00	76.84
23	2749 2750	CG OD1	ASP B ASP B	145	-6.159	28.159	21.614	1.00	84.39
	2751	OD2	ASP B ASP B	145 145	-6.061 -6.101	27.632	20.481	1.00	89.54
	2752	C	ASP B	145	-0.101 -7.434	29.394 25.135	21.801 23.618	1.00	78.78
	2753	Ö	ASP B	145	-6.468	24.371	23.546	1.00 1.00	72.65
30	2754	N	SER B	146	-8.423	24.971	24.496	1.00	66.12 68.40
	2755	CA	SER B	146	-B.445	23.857	25.441	1.00	59.96
	2756	CB	SER B	146	-9.433	24.128	26.579	1.00	59.40
	2757	og	SER B	146	-8.959	25.158	27.435	1.00	82.76
35	2758 2 7 59	C	SER B SER B	146	-8.862	22.590	24.725	1.00	55.02
23	2760	Ň	GLY B	146 147	-9.531 -8.462	22.649 21.447	23.703	1.00	74.05
	2761	ČA	GLY B	147	-8.811	20.174	25.267 24.662	1.00 1.00	55.86 55.22
	2762	C	GLY B	147	-7.680	19.168	24.739	1.00	55.22 55.94
40	2763	0	GLY B	147	-6.624	19.453	25.308	1.00	65.07
40	2764	N	THR B	148	-7.895	17.984	24.173	1.00	51.77
	2765	CA	THR B	148	-6.871	16.945	24.186	1.00	56.97
	2766 2767	CB OG1	THR B THR B	148	-7.493	15.537	24.299	1.00	62.53
	2768	CG2	THR B	148 148	-7.822 -8.769	15.054 15.581	22.992	1.00	93.22
45	2769	C	THR B	148	-6.061	17.028	25.130 22.895	1.00	61.98
	2770	Ō	THR B	148	-6.605	16.990	21.803	1.00 1.00	50.21 61.31
	2771	N	TYR B	149	-4.752	17.167	23.026	1.00	47.96
	2772	CA	TYR B	149	-3.873	17.263	21.870	1.00	36.15
50	2773	CB	TYR B	149	-2.907	18.438	22.008	1.00	39.15
50	2774 2775	CG CD1	TYR B TYR B	149	-3.504	19.814	21.873	1.00	32.57
	2776	CE1	TYR B	149 149	-4.170 -4.695	20.418	22.932	1.00	43.98
	2777	CD2	TYR B	149	-3.382	21.704 20.525	22.815 20.687	1.00	43.58
	2778	CE2	TYR B	149	-3.909	21.810	20.553	1.00 1.00	33.74 35.76
55	2779	CZ	TYR B	149	-4.564	22.396	21.621	1.00	41.82
	2780	ОН	TYR B	149	-5.089	23.668	21.494	1.00	40.18
	2781	Ç	TYR B	149	-3.028	16.013	21.730	1.00	38.28
	2782 2783	0	TYP B	149	-2.944	15.191	22.651	1.00	37.42
60	2784	N CA	TYR B TYR B	150	-2.386	15.893	20.573	1.00	28.35
00	2785	CB	TYR B	150 150	-1.500	14.776	20.287	1.00	32.70
	2786	CG	TYR B	150	-2.226 -3.180	13.421 13.018	20.440 19.328	1.00	46.79
	2787	CD1	TYR B	150	-2.710	12.397	18.168	1.00 1.00	40.91 38.70
	2788	CE1	TYR B	150	-3.588	12.007	17.150	1.00	49.78
65	2789	CD2	TYR B	150	-4.556	13.245	19.447	1.00	29.49
	2790	CE2	TYR B	150	-5.440	12.862	18.436	1.00	54.83
	2791	CZ	TYR B	150	-4.950	12.245	17.294	1.00	51.46
	2792 2793	C	TYR B	150	-5.828	11.857	16.310	1.00	68.38
70	2794	ŏ	TYR B TYR B	150 150	-1.002 -1.719	14.971 15.477	18.880	1.00	30.40
. •		-	5		-1.718	15.477	18.028	1.00	49.73

	2795	N	CYS B	15 i	0.241	14.596	18.645	4.00	
	2796	CA	CYS B	151	0.808	14.746	17.326	1.00	25.26
	2797	C	CYS B	151	1.175	13.410	16.699	1.00	39.72
	2798	ŏ	CYS B	151	1.270	12.395	17.383	1.00	37.05
5	2799	СВ	CYS B	151	2.040	15.652		1.00	49.88
•	2800	SG	CYS B	151	3.415		17.399	1.00	44.87
	2801	N	THR B	152		15.099	18.482	1.00	47.69
	2802	CA	THR B	152	1.380	13.419	15.387	1.00	34.36
	2803	CB			1.753	12 217	14.648	1.00	40.90
10	2804		THR B	152	0.641	11.715	13.712	1.00	46.04
10	2805	OG1	THR B	152	0.435	12.666	12.656	1.00	59.44
		CG2	THR B	152	-0.652	11.514	14.487	1.00	54.68
	2806	. С	THR B	152	2.906	12.646	13.784	1.00	39.86
	2807	0	THR B	152	3.063	13.845	13.500	1.00	42.60
15	2808	N	GLY B	153	3.707	11.680	13.355	1.00	28.17
15	2809	CA	GLY B	153	4.846	12.024	12. 540	1.00	26.12
	2810	С	GLY B	153	5.647	10.818	12,112	1.00	33.14
	2811	0	GLY B	153	5.622	9.753	12.734	1.00	34.08
	2812	N	LYS B	154	6.365	10.998	11.021	1.00	17.31
	2813	CA	LYS B	154	7.188	9.959	10.471	1.00	31.41
20	2814	CB	LYS B	154	7.185	17.086	8.949	1.00	
	2815	CG	LYS B	154	8.472	9.571	8.248	1.00	56.81
	2816	CD	LYS B	154	8.399	10.064	6.771		78.50
	2817	CE	LYS B	154	9.733	9.881	6.064	1.00	85.12
	2818	NZ	LYS B	154	9.649	10.343		1.00	88.41
25	2819	Ċ	LYS B				4.653	1.00	64.75
	2820	ŏ	LYS B	154	8.597	10.701	11.028	1.00	44.08
	2821	N		154	9.266	11.116	10.811	1.00	51.89
	2822			155	9.027	9.078	11.762	1.00	46.05
	2823	CA	VAL B	155	10.362	9.047	12.345	1.00	43.86
30	2824	CB	VAL B	155	10.321	8.903	13.878	1.00	37.35
20		CG1	VAL B	155	11.732	8.926	14.416	1.00	21.63
	2825	CG2	VAL B	155	9.487	10.030	. 14.499	1.00	48.98
	2826	C	VAL B	155	11.035	7.823	11.779	1.00	41.23
	2827	0	VAL B	155	10.560	6.716	11.989	1.00	37.63
25	2828	N	TRP B	156	12.129	8.012	11.057	1.00	52.20
35	2829	CA	TRP B	156	12.824	6.880	10.454	1.00	74.29
	2830	CB	TRP B	156	13.196	5.838	11.510	1.00	65.13
	2831	CG	TRP B	156	14.487	6.147	12.211	1.00	70.49
	2832	CD2	TRP B	156	15.771	6.221	11.629	1.00	54.80
	2833	CE2	TRP B	156	16.670	6.585	12.646	1.00	64.98
40	2834	CE3	TRP B	156	16.252	6.012	10.334	1.00	50.71
	2835	CD1	TRP B	156	14.631	6.458	13.539	1.00	71.39
	2836	NE1	TRP B	156	15.954	6.725	13.804	1.00	
	2837	CZ2	TRP B	156	18.051	6.752	12.415	1.00	63.30
	2838	CZ3	TRP B	156	17.624	6.179	10.101	1.00	62.21
45	2839	CH2	TRP B	156	18.500	6.545	11.141	1.00	67.16
	2840	C	TRP B	156	12.015	6.201	9.347		53.68
	2841	ŏ	TRP B	156	11.962	4.971		1.00	90.81
	2842	Ň	GLN B	157	11.389	7.013	9.263	1.00	111.59
	2843	CA	GLN B	157	10.608	6.526	8.506	1.00	88.48
50	2844	CB	GLN B	157	11.461		7.382	1.00	85.04
	2845	CG	GLN B	157		5.575 5.304	6.536	1.00	110.53
	2846	CD	GLN B		10.930	5.324	5.138	1.00	124.62
	2847	OE1		157	11.824	4.383	4.337	1.00	129.56
	2848	NE2	GLN B	157	12.951	4.080	4.749	1.00	127.90
55	2849		GLN B	157	11.329	3.926	3.183	1.00	123.80
33	2850	C	GLN B	157	9.311	5.842	7.816	1.00	78.48
		0	GLN B	157	8.544	5.392	6.977	1.00	77.35
	2851	N	LEU B	_. 158	9.074	5.760	9.122	1.00	70.67
	2852	CA	LEU B	158	7.849	5.147	9.635	1.00	70.41
60	2853	CB	LEU B	158	8.170	4.049	10.637	1.00	81.95
60	2854	CG	LEU B	158	8.646	2.722	10.055	1.00	86.23
	2855	CD1	LEU B	158	8.865	1.715	11.174	1.00	105.28
	2856	CD2	LEU B	158	7.602	2.204	9.081	1.00	94.27
	2857	С	LEU B	158	6.998	6.203	10.313	1.00	70.44
	2858	0	LEU B	158	7.499	7.275	10.632	1.00	80.05
65	2859	N	ASP B	159	5.721	5.904	10.537	1.00	67.41
	2860	CA	ASP B	159	4.837	6.880	11.171	1.00	82.00
	2861	CB	ASP B	159	3.519	7.001	10.392	1.00	
	2862	CG	ASP B	159	3.736	7.375	8.938		86.28
_	2863	OD1	ASP B	159	4.285	8.469	8.664	1.00	106.10
70	2864	OD2	ASP B	159	3.361	6.564	8.067	1.00	117.95
		- 			0.001	· ·	0.007	1.00	115.39

	2865	С	ASP B	159	4.547	6.495	12.611	1.00	77 10
	2866	0	ASP B	159	4.590	5.316	12.962	1.00	77.19 77.19
	2867	N	TYR B	160	4,274	7.492	13.448	1.00	65.57
5	2868	CA	TYR B	160	3.972	7.232	14.842	1.00	48.77
,	2869 2870	CB CG	TYR B TYR B	160	5.244	7.273	15.670	1.00	37.12
	2871	CD1	TYR B	160 160	6.332 7.199	6.371 6.797	15.148	1.00	34.46
	2872	CE1	TYR B	160	8.195	5.961	14.134 13.645	1.00	37.79
	2873	CD2	TYR B	160	6.490	5.086	15.661	1.00 1.00	56.87
10	2874	CE2	TYR B	160	7.486	4.233	15.179	1.00	19.69 40.99
	2875	CZ	TYR B	160	8.341	4.674	14.172	1.00	60.40
	2876	он	TYR B	160	9.343	3.841	13.702	1.00	70.89
	2877 2878	C	TYR B TYR B	160	3.000	8.266	15.364	1.00	54.13
15	2879	Ň	GLU B	160 161	2.718 2.496	9.265	14.687	1.00	60.44
	2880	ČA	GLU B	161	1.546	8.022 8.926	16.569 17.193	1.00	47.74
	2881	СВ	GLU B	161	0.133	8.387	16.988	1.00	48.57 55.17
	2882	CG	GLU B	161	-0.965	9.106	17.748	1.00	80.84
20	2883	CD	GLU B	161	-2.360	8.757	17.226	1.00	93.70
20	2884 2885	OE1	GLU B	161	-3.352	9.054	17.932	1.00	99.33
	2886	⊃E2 C	GLU B GLU B	161	-2.465	8.198	16.106	1.00	101.86
	2887	ŏ	GLU B	161 161	1.872 2.080	9.038 8.028	18.671	1.00	56.41
	2888	Ň	SER B	162	1.928	10.268	19.340 19.173	1.00 1.00	58.09
25	2889	CA	SER B	162	2.240	10.515	20.578	1.00	61.15 70.01
•	2890	CB	SER B	162	2.700	11.965	20.771	1.00	82.47
	2891	OG	SER B	162	1.646	. 12.889	20.523	1.00	75.43
	2892 2893	C	SER B SER B	162	1.046	10.258	21.481	1.00	69.94
30	2894	O N	GLU B	162 163	-0.083	10.163	21.017	1.00	70.40
50	2895	CA	GLU B	163	1.301 0.223	10.133 9.924	22.776 23.728	1.00	76.24
	2896	CB	GLU B	163	0.785	9.585	25.106	1.00 1.00	74.01 83,42
	2897	CG	GLU B	163	1.437	8.222	25.201	1.00	108.95
35	2898	CD	GLU B	163	0.421	7.096	25.165	1.00	124.63
22	2899 2900	OE1 OE2	GLU B	163	-0.463	7.070	26.051	1.00	126.10
	2901	C	GLU B GLU B	163 163	0.507 -0.517	6.239	24.255	1.00	137.68
	2902	ŏ	GLU B	163	-0.517 0. 09 6	11.246 12.303	23.809 23.836	1.00 \ 1.00	64.66
	2903	Ň	PRO B	164	-1.848	11.211	23.829	1.00	78.89 49.91
40	2904	CD	PRO B	164	-2.763	10.066	23.886	1.00	45.53
	2905	CA	PRO B	164	-2.580	12.477	23.912	1.00	49.79
	2906 2907	CB CG	PRO B	164	-4.040	12.042	23.913	1.00	50.14
	2908	C	PRO B PRO B	164 164	-3.988	10.692	24.532	1.00	54.43
45	2909	ŏ	PRO B	164	-2.210 ` -1. 6 76	13.229 12.650	25.177 26.121	1.00 1.00	52.68
	2910	N	LEU B	165	-2.496	14.523	25.187	1.00	55.25 46.01
	2911	CA	LEU B	165	-2.195	15.363	26.330	1.00	38.63
	2912	CB	LEU B	165	-0.862	16.080	26.112	1.00	42.39
50	2913 2914	CG CD1	LEU B LEU B	165	-0.390	17.012	27.232	1.00	34.72
50	2915	CD1 CD2	LEU B LEU B	165 165	0.058 0.765	16.181	28.423	1.00	36.79
	2916	C	LEU B	165	-3. 30 6	17.879 16.390	26.732	1.00	31.18
	2917	Ö	LEU B	165	-3.561	17.181	26.491 25.597	1.00 1.00	41.11 47.00
	2918	N	ASN B	166	-3.983	16.369	27.626	1.00	47.91
55	2919	CA	ASN B	166	-5.044	17.332	27 352	1.00	62.56
	2920 2921	CB	ASN B	166	-5.919	16.892	29.031	1.00	89.42
	2922	CG OD1	ASN P ASN B	166	-6.897	15.795	28.644	1.00	111.40
	2923	ND2	ASN B	166 166	-7.511 -7.069	15.874 14.782	27.581	1.00	117.56
60	2924	C	ASN B	166	-4.419	18.685	29.490 28.139	1.00 1.00	128.12 63.19
	2925	0	ASN B	166	-3.385	18.758	28.798	1.00	75.62
	2926	N	ILE B	167	-5.028	19.743	27.614	1.00	55.85
	2927	CA	ILE B	167	-4.547	21.103	27.837	1.00	50.63
65	2928 2929	CB CG2	ILE B	167	-3.775	21.642	26.625	1.00	41.65
00	2930	CG1	ILE B ILE B	167 167	-3.644	23.158	26.704	1.00	27.67
	2931	CD1	ILE B	167	-2.398 -1.576	20.981 21.401	26.572 25.373	1.00	49.69
	2932	C	ILE B	167	-5.719	22.018	25.373 28.127	1.00 1.00	71. 73 52.51
70	2933	0	ILE B	167	-6.636	22.141	27.328	1.00	54.25
70	2934	N	THR B	168	-5.677	22.669	29.279	1.00	62.54

	2935 2936	CA CB	THR B	168 168	-6.762 -7.371	23.552 23.090	29.672 30.995	1.00 1.00	73.12 77.82
	2937	OG1	THR B	168	-7.229	21.668	31.116	1.00	71.03
5	2938 2939	CG2	THR B	168	-8.847	23.472	31.049	1.00	80.41
,	2940	CO	THR B	168	-6.329	25.002	29.841	1.00	79.24
	2941	Ň	THR B VAL B	168 169	-5.347 -7.070	25.294 25.007	30.526	1.00	81.73
	2942	CA	VAL B	169	-7.070 -6.792	25.907 27.336	29.214	1.00	81.68
	2943	CB	VAL B	169	-6.787	27.996	29.302	1.00	82.56
10	2944	CG1	VAL B	169	-6.538	29.487	27.916 28.048	1.00	80.42
	2945	CG2	VAL B	169	-5.731	27.352	27.041	1.00 1.00	71.55
	2946	C	VAL B	169	-7.937	27.908	30.115	1.00	82.46 89.49
	2947	0	VAL B	169	-9.098	27.841	29.696	1.00	87.82
	2948	N	ILE B	170	-7.625	28,469	31.277	1.00	94.48
15	2949	CA	ILE B	170	-8.668	28.995	32.143	1.00	101.94
	2950	CB	ILE B	170	-8.332	28.730	33.631	1.00	98.82
	2951	CG2	ILE B	170	-8.574	27.262	33.966	1.00	99.33
	2952	CG1	ILE B	170	-6.876	29.092	33.912	1.00	103.85
20	2953 2954	CD1	ILE B	170	-6.453	28.836	35.347	1.00	102.26
20	2954 2955	C	ILE B	170	-9.027	30.467	31.967	1.00	106.09
	2956	N.I.	LYS B	170 171	-8.162	31.307	31.727	1.00	103.79
	2957	CA T	LYS B	171	-10.326 -10.870	30.715 32.069	32.066	1.00	115.25
	2958	CB	LYS B	171	-12.374	32.030	32.000	1.00	116.92
25	2959	ČĞ	LYS B	171	-13.021	33,402	31.674 31.721	1.00	111.37
	2960	CD	LYS B	171	-12.523	34.293	30.594	1.00 1.00	106.02
	2961	CE	LYS B	171	-13.256	35.629	30.587	1.00	110.98
	2962	NZ	LYS B	171	-12.673	36.579	29.609	1.00	109.27 99.03
	2963	С	LYS B	171	-10.606	32.682	33.357	1.00	122.05
30	2964	0	LYS B	171	-10.455	31.952	34.327	1.00	122.45
	2965	N	ALA B	172	-10.550	34.004	33.492	1.00	121.93
	2966	CA	ALA B	172	-10.154	34.550	34.807	1.00	124.78
	2967	CB	ALA B	172	-8.778	35.182	34.669	1.00	110.24
35	2968	C	ALA B	172	-11.069	35.577	35.528	1.00	131.95
33	2969 2970	O N	ALA B	172	-11.006	36.782	35,303	1.00	136.47
	2971	CD	PRO B PRO B	173	-11.911	35.025	36.361	1.00	138.57
	2972	CA	PRO B	173 173	-12.775	34.002	35.754	1.00	133.76
	2973	CB	PRO B	173	-12.781 -13.714	35.842 34.799	37.272 37.970	1.00	145.56
40	2974	CG	PRO B	173	-13.935	33.894	37.872 36.705	1.00	143.51
	2975	Č	PRO B	173	-12.008	36.690	38.273	1.00 1.00	139.83 152.09
	2976	0	PRO B	173	-10.896	36.332	38.614	1.00	158.41
	2977	N	ARG B	174	-12.559	37.804	38.749	1.00	156.36
	2978	CA	ARG B	174	-11.852	38.646	39.733	1.00	159.88
45	2979	CB	ARG B	174	-10.934	39.640	39.008	1.00	160.37
	2980	CG	ARG B	174	-11.660	40.518	38.000	1.00	164.23
	2981	CD	ARG B	174	-11.074	40.350	36.593	1.00	169.49
	2982 2983	NE	ARG B	174	-12.049	40.638	35.539	1.00	176.01
50	2984	CZ NH1	ARG B	174	-12.039	41.731	34.773	1.00	180.58
30	2985	NH2	ARG B ARG B	174	-11.100	42.655	34.956	1.00	179.79
-	2986	C	ARG B	174 174	-12.954 -12.853	41.882	33.824	1.00	181.42
	2987	ŏ	ARG B	174		39.368 38.809	40.639	1.00	160.54
	2988	Č1	NAG B	221	-13.891 22.996	15.148	41.006	1.00	159.92
55	2989	C2	NAG B	221	23.132	14.494	29.775 28.397	1.00	90.21 106.23
	2990	N2	NAG B	221	21.968	13.691	28.083	1.00 1.00	110.50
	2991	C7	NAG B	221	21.087	14,132	27.187	1.00	10.50
	2992	07	NAG B	221	21.209	15.211	26.594	1.00	98.37
	2993	C8	NAG B	221	19.888	13.243	26.902	1.00	105.30
60	2994	C3	NAG B	221	24.395	13.644	28.376	1.00	115.44
	2995	03	NAG B	221	24.547	13.046	27.097	1.00	116.65
	2996	C4	NAG B	221	25.598	14.538	28.682	1.00	118.34
	2997	O4	NAG B	221	26.785	13.757	28.731	1.00	122.24
65	2998 2999	C5	NAG B	221	25.393	15.264	30.022	1.00	113.54
0 5	3000	O5 Ce	NAG B	221	24.136	15.989	30.028	1.00	102.61
	3000	C6 O6	NAG B	221	26.494	16.278	30.269	1.00	108.41
	3002	C1	NAG B	221	26.454	16.766	31.601	1.00	119.03
	3003	62	ŅAG B NAG B	242 242	7.596 8.393	9.421	42.304	1.00	89.99
70	3004	N2	NAG B	242	9.815	8.151 8.410	42.040 42.148	1.00	87.43
·		<u>-</u>			0.010	J.+10	76.140	1.00	86.29

	3005	C7 O7	NAG B	242	10.433	8.308	43.321	1.00	82.76
	3006		NAG B	242	9.852	7.998	44.367	1.00	76.22
	3007 3008	ය	NAG B	242	11.928	8.599	43.333	1.00	77.25
5	3009	∝ os	NAG B NAG B	242 242	8.059	7.652	40.641	1.00	90.08
,	3010	ος C4	NAG B	242 242	8.693 6.539	6.400 7.501	40.436	1.00	97.55
	3011	34	NAG B	242 242	6.283	7.380	40.426	1.00	91.14
	3012	C5	NAG B	242	5.757	8.728	39.009 40.956	1.00	112.32
	3013	O5	NAG B	242	6.202	9.104	42.276	1.00	82.98
10	3014	C6	NAG B	242	4.266	8.467	41.060	1.00	91.07
	3015	06	NAG B	242	3.514	9.640	40.779	1.00 1.00	84.52
	3016	C1	NAG B	243	6.193	6,123	38.423	1.00	85.63 105.62
	3017	C2	NAG B	243	5.464	6.267	37.081	1.00	105.62
	3018	N2	NAG B	243	4.122	6.776	37.289	1.00	107.52
15	3019	C7	NAG B	243	3.804	7.995	36.858	1.00	90.92
	3020	Q 7	NAG B	243	4.599	8.719	36.255	1.00	78.67
	3021	C8	NAG B	243	2.389	8.483	37.120	1.00	83.10
	3022	C3	NAG B	243	5.435	4.929	36.344	1.00	112.30
	3023	O3	NAG B	243	4.817	5.094	35.073	1.00	112.99
20	3024	C4	NAG B	243	6.875	4.455	36.166	1.00	114.52
	3025	04	NAG B	243	6.914	3.184	35.480	1.00	130.57
	3026	C5	NAG B	243	7.570	4.361	37.533	1.00	107.51
	3027	O5	NAG B	243	7.529	5.646	38.195	1.00	110.47
25	3028	C6	NAG B	243	9.034	3.978	37.402	1.00	100.22
23	3029	O6	NAG B	243	9.696	3.984	38.659	1.00	87.89
	3030	C1	MAN B	244	7.657	3.203	34.307	1.00	139.64
	3031 3032	C2 O2	MAN B	244	0.//2	2.971	33.058	1.00	140.01
	3033	C3	MAN B MAN B	244	7.304	3.675	31.948	1.00	144.21
30	3034	og Og	MAN B	244 244	6.590 6.103	1.496 1.414	32.679	1.00	138.91
50	3035	24	MAN B	244	7.910	0.735	31.347	1.00	144.28
	3036	04	MAN B	244	7.708	-0.643	32. 788 32.517	1.00 1.00	139.81
	3037	C5	MAN B	244	8.435	0.909	34.198	1.00	144.34 140.48
	3038	O5	MAN B	244	8.779	2.294	34.406	1.00	147.09
35	3039	C6	MAN B	244	9.676	0.070	34.479	1.00	136.69
	3040	O6	MAN B	244	10.863	0.718	34.041	1.00	123.90
	3041	C1	NAG B	335	10.916	24.720	18.959	1.00	65.94
	3042	C2	NAG B	33 5	12.028	24.987	17.932	1.00	79.27
40	3043	N2	NAG B	335	11.848	24.183	16.736	1.00	91.33
40	3044	C7	NAG B	335	11.340	24.727	15.629	1.00	98.55
	3045	07	NAG B	335	10.962	25.902	15.560	1.00	81.86
	3046	C8	NAG B	335	11.212	23.824	14.411	1.00	99.41
	3047 3048	C3	NAG B	335	13.413	24.705	18.548	1.00	84.72
45	3048	03 C4	NAG B	335	14.442	25.019	17.611	1.00	91.27
40	3050	ζ 4 04	NAG B NAG B	335	13.604	25.515	19.838	1.00	80.89
	3051	C5	NAG B	335 335	14.831	25.090 25.095	20.488	1.00	64.07
	3052	O5	NAG B	335	12.419	25.265 25.538	20.794	1.00	64.08
	3053	C6	NAG B	335	11.144 12.531	25.538 26.144	20.131	1.00	71.94
50	3054	Ŏ6	NAG B	335	11.291	26.809	22.030 22.362	1.00	64.49
	3055	C1	NAG B	336	15.929	25.939	20.563	1.00 1.00	45.77
	3056	C2	NAG B	336	16.577	25.748	21.946	1.00	97.76 97.78
	3057	N2	NAG B	336	15.705	26.270	22.982	1.00	97.76 97.76
	3058	C7	NAG B	336	15.077	25.437	23.810	1.00	97.93
55	3059	07	NAG B	336	15.179	24.203	23.741	1.00	97.68
	3060	C8	NAG B	336	14.193	26.073	24.873	1.00	97.92
	3061	C3	NAG B	336	17.943	26.425	22.064	1.00	97.90
	3062	03	NAG B	336	18.571	25.981	23.258	1.00	98.29
60	3063	C4	NAG B	336	18.847	26.092	20.880	1.00	98.00
60	3064	Q4	NAG B	336	20.012	26.915	20.922	1.00	97.87
	3065	C5	NAG B	336	18.103	26.315	19.557	1.00	97.95
	3066	O5	NAG B	336	16.862	25.561	19.525	1.00	97.83
	3067	C6	NAG B	336	18.956	25.835	18.400	1.00	97.91
65	3068	O6	NAG B	336	18.216	25.798	17.193	1.00	97.89
w	3069	C1	FCA B	337	11.537	27.883	23.223	1.00	97.62
	3070	C2	FCA B	337	10.367	28.129	24.189	1.00	97.53
	3071 3072	C3 C4	FCA B	337	9.202	28.823	23.571	1.00	97.82
	3072	C4 C5	FCA B	337	9.595	30.213	22.961	1.00	97.76
70	3074	C6	FCA B FCA B	337 337	10.713	29.895	21.926	1.00	97.77
. •	JU/ T	•	FUA D	337	11.421	31.110	21.306	1.00	97.74

	0000		504 0						
	3075	02	FCA B	337	9.934	26.823	24.727	1.00	97.69
	3076	03	FCA B	337	8.162	29.022	24.541	1.00	97.99
	3077	04	FCA B	337	10.062	31.100	24.005	1.00	97.77
5	3078	O5	FCA B	337	11.775	29.137	22.508	1.00 •	97.61
3	3079	C1	NAG B	340	-0.412	38.735	24.336	1.00	122.51
	3080	C2	NAG B	340	-1.134	39.580	25.381	1.00	120.32
	3081	N2	NAG B	340	-2.513	39.812	24.998	1.00	123.12
	3082	C7	NAG B	340	-3.481	39.652	25.892	1.00	119.35
10	3083	07	NAG B	340	-3.272	39.289	27.048	1.00	117.53
10	3084	C8	NAG B	340	-4.900	39.928	25.422	1.00	119.54
	3085	C3	NAG B	340	-0.418	40.906	25.454	1.00	119.27
	3086	O3	NAG B	340	-1.096	41.797	26.326	1.00	109.33
	3087	C4	NAG B	340	1.035	40.774	25.885	1.00	127.45
٠,٠	3088	Q 4	NAG B	340	1.546	42.148	25.882	1.00	140.24
15	3089	C5	NAG B	340	1.739	39.801	24.880	1.00	128.90
	3090	O5	NAG B	340	0.965	38.548	24.746	1.00	126.48
	3091	C6	NAG B	340	3.135	39.394	25.344	1.00	127.49
	3092	O6	NAG B	340	3.474	38.081	24.908	1.00	123.34
00	3093	C1	NAG B	341	2.837	42.676	25.784	1.00	149.17
20	3094	C2	NAG B	341	3.740	42.731	27.002	1.00	145.12
	3095	N2	NAG B	341	2.968	42.757	28.228	1.00	146.42
	3096	C7	NAG B	341	2.704	41.612	28.847	1.00	145.07
	3097	07	NAG B	341	3.106	40.526	28.416	1.00	132.12
0.5	3098	C8	NAG B	341	1.890	41.672	30.122	1.00	142.75
25	3099	C3	NAG B	341	4.552	44.017	26.806	1.00	143.92
	3100	O3	NAG B	341	5.474	44.200	27.872	1.00	142.89
	3101	C4	NAG B	341	5.304	43.958	25.449	1.00	148.66
	3102	04	NAG B	341	5.954	45.201	25.210	1.00	144.18
-	3103	C5	NAG B	341	4.351	43.643	24.269	1.00	155.68
30	3104	O5	NAG B	341	3.515	42.481	24.540	1.00	161.36
	3105	C6	NAG B	341	5.092	43.354	22.983	1.00	161.88
	3106	O6	NAG B	341	4.581	44.135	21.915	1.00	165.58
	3107	C1	NAG B	366	-8.147	13.841	29.242	1.00	143.91
~~	3108	C2	NAG B	366	-8.310	12.851	30.401	1.00	148.60
35	3109	N2	NAG B	366	-7.063	12.152	30.649	1.00	155.49
	3110	C7	NAG B	366	-6.400	12.345	31.787	1.00	156.20
	3111	07	NAG B	366	-6.791	13.114	32.670	1.00	152,95
	3112	C8	NAG B	366	-5.103	11.570	31.975	1.00	155.57
40	3113	C3	NAG B	366	-9.420	11.849	30.045	1.00	149.01
40	3114	03	NAG B	366	-9.658	10.967	31.133	1.00	143.79
	3115	C4	NAG B	366	-10.713	12.593	29.696	1.00	151.07
	3116	04	NAG B	366	-11.684	11.663	29.237	1.00	149.83
	3117	C 5	NAG B	366	-10.447	13.654	28.611	1.00	149.31
4.5	3118	O5	NAG B	366	-9.380	14.536	29.019	1.00	146.79
45	3119	C6	NAG B	366	-11.657	14.529	28.340	1.00	149.54
	3120	O6	NAG B	366	-11.370	15.902	28.578	1.00	136.69

Table 8. Atomic coordinates of PhFcεRIα₁₋₁₇₂, Form H1

	ATOM NUMBER	ATOM TYPE	RESIDUE		_x_	Υ	_ z	<u>occ</u>	ь
	•	СВ	MAL	_					<u>B</u>
5	1 2	CG1	VAL VAL	1	53.051 52.370	36.792 35.571	77.715	1.00	118.55
_	3	CG2	VAL	i	53.204	37.651	77.956 79.132	1.00 1.00	118.55
	4	C	VAL	1	54,467	36.682	75.485	1.00	118.55 75.78
	5	0	VAL	1	53.770	37.511	74.950	1.00	75.78
10	6 7	N	VAL	1	55.482	37.216	77.849	1.00	75.78
10	8	CA N	VAL PRO	1	54.432	36.462	77.091	1.00	75.78
	9	CD	PRO	2	55.312 56.277	35.953 34.989	74.688 75.182	1.00	130.31
	10	CA	PRO	2 2 2 2 2 2 3	55.477	36.015	73.216	1.00 1.00	94.32
. ~	11	СВ	PRO	2	56.190	34.719	72.910	1.00	130.31 94.32
15	12	CG	PRO	2	57.105	34.684	74.012	1.00	94.32
	13	C	PRO	2	54.053	36.005	72. 7 06	1.00	130.31
	14 15	0 N	PRO GLN	2	53.189	35.367	73.293	1.00	130.31
	16	CA	GLN	3	53.786 52.463	36.805 36.918	71.691	1.00	104.92
20	17	CB	GLN	3	52.537	37.847	71.130 69.919	1.00 1.00	104.92
	18	CG	GLN	3	51.192	38.291	69.421	1.00	99.07 99.07
	19	CD	GLN	3	50.249	38.740	70.542	1.00	99.07
	20	OE1	GLN	3	50.548	39.683	71.287	1.00	99.07
25	21 · · · · · · · · · · · · · · · · · · ·	NE2	GLN	3	49.101	38.061	70.664	1.00	99.07
23	23	CO	GLN GLN	3 3	52.005	35.499	70.762	1.00	104.92
	24	Ň	LYS	4	52.779 50.747	34.545 35.334	70.877	1.00	104.92
	25	CA	LYS	4	50.255	33.998	70.360 69.981	1.00 1.00	70.29
~~	26	CB	LYS	4	48.731	33.942	70.002	1.00	70.29 91.56
30	27	CG	LYS	4	47.997	34.836	69.020	1.00	91.56
	28	CD	LYS	4	46.591	34.284	68.830	1.00	91.56
	29 30	CE NZ	LYS LYS	4	45.661	35.309	68.214	1.00	91.56
	31	C	LYS	4	45.296 50.735	36.401 33.524	69.165	1.00	91.56
35	32	ŏ	LYS	4	50.793	34.314	68.613 67.654	1.00 1.00	70.29
	33	N	PRO	5	51.056	32.216	68.503	1.00	70.29 78.97
	34	CD	PRO	5	51.154	31.280	69.633	1.00	108.62
	35	CA	PRO	5	51.541	31.566	67.284	1.00	78.97
40	36 37	CB CG	PRO PRO	5	51.808	30.127	67.739	1.00	108.62
-10	38	C	PRO	5 5	52.211 50.601	30.315 31.638	69.151	1.00	108.62
	39	ŏ	PRO	5	49.439	32.036	66.091 66.221	1.00	78.97
	40	N	LYS	6	51.124	31.294	64.916	1.00 1.00	78.97 88.04
15	41	CA	LYS	6	50.283	31.336	63.731	1.00	88.04
45	42	CB	LYS	6	50.440	32.681	63.010	1.00	139.11
	43 44	CG CD	LYS	6	49.189	33.108	62.233	1.00	i39.11
	45	CE	LYS LYS	6 6	49.300	34.555	61.830	1.00	139.11
	46	NZ	LYS	6	47.998 48.130	35.105 36.569	61.293 61.033	1.00	139.11
50	47	c	LYS	6	50.598	30.191	62.780	1.00 1.00	139.11 88.04
	48	0	LYS	6	51.765	29.850	62.565	1.00	88.04
	49	N	VAL	7	49.539	29.590	62.235	1.00	50.50
	50 51	CA	VAL	7	49.660	28.476	61.307	1.00	50.50
55	52	CB CG1	VAL VAL	7 7	48.471	27.522	61.411	1.00	69.58
J J	53	CG2	VAL	7	48.757 48.212	26.276 27.169	60.577	1.00	69.58
	54	C	VAL	7	49.733	28.947	62.858 59.871	1.00 1.00	69.58
	55	0	VAL	7	48.997	29.831	59.446	1.00	50.50 50.50
۲0	56	N	SER	8	50.597	28.301	59.112	1.00	106.26
60	57 50	CA	SER	8	50.788	28.646	57.723	1.00	106.26
	58 59	CB OG	SER	8	52.121	29.344	57.568	1.00	69.57
	60	C	SER SER	8 8	53.155 50.816	28.427	57.902	1.00	69.57
	61	ŏ	SER	8	51.370	27,357 26,353	56.933 57.280	1.00	106.26
65	62	Ň	LEU	9	50.221	27.381	57.380 55.754	1.00 1.00	106.26 69.51
	63	CA	LEU	9	50.212	26.187	54.937	1.00	69.51 69.51
	64	CB	LEU	9	48.809	25.862	54.432	1.00	46.80
				•				-	

	65 66	CG CD1	LEU	. 9 ·	47.549 46.349	26.374 25.850	55.111 54.373	1.00 1.00	46.80 46.80
	67	CD2	LEU	9	47.523	25.926	56.559	1.00	46.80
5	68	C	LEU	9	51.111	26.317	53.718	1.00	69.51
5	69 70	O N	LEU ASN	9	51.229	27.385	53.110	1.00	69.51
	71	ČA	ASN	10 10	51.725 52.576	25.199 25.120	53.358	1.00	65.02
	72	CB	ASN	10	54.050	25.120 25.035	52.197 52.622	1.00	65.02
	73	ČĠ	ASN	10	54.979	24.700	51.475	1.00 1.00	82.93
10	74	OD1	ASN	10	54.991	25.378	50.451	1.00	82.93 82.93
	75	ND2	ASN	10	55.771	23.650	51.643	1.00	82.93
	76	С	ASN	10	52.130	23.839	51.492	1.00	65.02
	77	0	ASN	10	52.431	22.728	51.953	1.00	65.02
15	78	N	PRO	11	51.306	23.967	50.430	1.00	60.91
13	79 80	CD CA	PRO PRO	11	50.772	22.738	49.827	1.00	59.89
	8;	CB	PRO	11 11	50.786	25.157	49.733	1.00	60.91
	82	CG	PRO	11	49.977 50.471	24.568	48.583	1.00	59.89
	83	č	PRO	11	49.881	23.159 26.032	48.449 50.613	1.00	59.89
20	84	O	PRO	!1	49.435	25 ~ '8	51.675	1.00 1.00	60.91 60.91
	85	N	PRO	1.2	49.570	27.245	50.142	1.00	78.15
	86	CD	PRO	12	50.133	27.764	48.895	1.00	41.22
	87	CA	PRO	12	48.728	28.264	50.791	1.00	78.15
25	88	СВ	PRO	12	48.984	29.528	49.967	1.00	41.22
23	89 90	ce	PRO	12	50.225	29.226	49.207	1.00	41.22
	90 91	C	PRO PRO	12	47.264	27.890	50.704	1.00	78.15
	92	N	TRP	12 13	46.420	28.401	51.437	1.00	78.15
	93	CA	TRP	13	46.975 45.621	27.001	49.773	1.00	63.58
30	94	CB	TRP	13	45.619	26.563 25.679	49.541	1.00	63.58
	95	CG	TRP	13	46.483	26.211	48.308 47.211	1.00 1.00	43.81
	96	CD2	TRP	13	46.444	27.519	46.634	1.00	43.81 43.81
	97	CE2	TRP	13	47.339	27.524	45.549	1.00	43.81
25	98	CE3	TRP	13	45.732	28.687	46.926	1.00	43.81
35	99	CD1	TRP	13	47.385	25.507	46.480	1.00	43.81
	100	NE1	TRP	13	47.903	26.281	45.477	1.00	43.81
	101 102	CZ2 CZ3	TRP	13	47.543	28.650	44.746	1.00	43.81
	103	CH2	TRP TRP	13 13	45.935 46.838	29.812	46.128	1.00	43.81
40	104	Č	TRP	13	45.032	29.780 25.822	45.046	1.00	43.81
	105	Ö	TRP	13	45.556	24.777	50.730 51.137	1.00 1.00	63.58 63.58
	106	N	ASN	14	43.947	26.377	51.280	1.00	73.67
	107	CA	ASN	14	43.239	25.781	52.412	1.00	73.67
45	108	CB	ASN	14	42.720	26.868	53.362	1.00	86.63
45	109	CG	ASN	14	41.638	27.726	52.745	1.00	86.63
	110 111	OD1	ASN	14	41.780	28.226	51.630	1.00	86.63
	112	ND2 C	ASN	14	40.548	27.912	53.477	1.00	86.63
	113	ŏ	ASN ASN	14 14	42.090	24.940	51.861	1.00	73.67
50	114	Ň	ARG	15	41.276 42.045	24.409 24.837	52.609	1.00	73.67
	115	ĊA	ARG	15	41.058	24.054	50.534 49.800	1.00 1.00	50.70
	116	CB	ARG	15	40.174	24.947	48.943	1.00	50.70 57.52
	117	CG	ARG	15	39.558	26.093	49.674	1.00	57.52
<i>E E</i>	118	CD	ARG	15	38.636	26.850	48.745	1.00	57.52
55	119	NE	ARG	15	37.242	26.435	48.833	1.00	57.52
	120	cz	ARG	15	36.364	26.620	47.853	1.00	57.52
	121 122	NH1	And	15	36.752	27.189	46.730	1.00	57.52
	123	NH2 C	ARG	15	35.093	26.286	47.999	1.00	57.52
60	124	ŏ	ARG ARG	15 15	41.851	23.139	48.858	1.00	50.70
	125	Ň	ILE	. 16	42.427 41.902	23.596 21.849	47.863	1.00	50.70
	126	ĊA	ILE	16	42.633	20.980	49.150 48.254	1.00 1.00	58.15 58.15
	127	CB	ILE	16	43.956	20.548	48.866	1.00	58.15 51.72
	128	CG2	ILE	16	44.934	21.703	48.821	1.00	51.72
65	129	CG1	ILE	16	43.718	20.052	50.287	1.00	51.72
	130	CD1	ILE	16	44.968	19.557	50.978	1.00	51.72
	131 132	C	ILE	16	41.839	19.761	47.876	1.00	58.15
	132	0 N	ILE	16	40.875	19.403	48.540	1.00	58.15
70	134	ÇA	PHE	17 17	42.260	19.157	46.776	1.00	58.19
. •		₩	rne	'' .	41.660	17.957	46.241	1.00	58.19

	135 136	CB CG	PHE PHE	17 · 17	42.213 41.536	17.669 18.414	44.860 43.776	1.00	25.51
	137	CD1:	PHE	17	42.250	18.820	42.639	1.00 1.00	25.51
_	138	CD2	PHE	17	40.171	18.682	43.857	1.00	25.51 25.51
5	139	CE1	PHE	17	41.608	19.487	41.592	1.00	25.51
	140	CE2	PHE	17	39.532	19.344	42.825	1.00	25.51
	141 142	CZ C	PHE	17	40.253	19.752	41.673	1.00	25.51
	143	ŏ	PHE PHE	17 17	42.019	16.789	47.117	1.00	58.19
10	144	Ň	LYS	18	43.030 41.202	16.815 15.749	47.836 47.024	1.00	58.19
	145	CA	LYS	18	41.421	14.528	47.770	1.00 1.00	64.21
	146	CB	LYS	18	40.266	13.572	47.476	1.00	64.21 120.30
	147	CG	LYS	18	40.180	12.351	48.352	1.00	120.30
15	148	CD	LYS	18	38.856	11.639	48.078	1.00	120.30
13	149 150	CE NZ	LYS LYS	18	38.656	10.437	48.983	1.00	120.30
	151	Č	LYS	18 18	39.547 42.740	9.324 13.978	48.594	1.00	120.30
	152	ŏ	LYS	18	42.970	13.995	47. 23 7 46.027	1.00	64.21
	153	N	GLY	19	43.619	13.536	48.134	1.00 1.00	64.21 59.20
20	154	CA	GLY	19	44.893	12.963	47.706	1.00	59.20
	155	C	GLY	19	46.112	13.851	47.506	1.00	59.20
	156	0 N	GLY	19	47.199	13.352	47.174	1.00	59.20
	157 158	CA	GLU GLU	20 20	45.938 47.046	15.156	47.686	1.00	96.38
25	159	CB	GLU	20	47.046 46.547	16.087 17.429	47.539 46.000	1.00	96.38
	160	ČĠ	GLU	20	45.820	17.303	46.993 45.661	1.00 1.00	62.66
	161	CD	GLU	20	45.468	18.648	45.025	1.00	62.66 62.66
	162	OE1	GLU	20	44.899	19.525	45.726	1.00	62.66
30	163	OE2	GLU	20	45.754	18.811	43.815	1.00	62.66
30	164 165	CO	GLU GLU	20 20	47.666	16.261	48.917	1.00	96.38
	166	Ň	ASN	20	47.055 48.886	15.899 16.783	49.922	1.00	96.38
	167	CA	ASN	21	49.550	16.992	48.966 50.245	1.00 1.00	82.14 82.14
~~	168	CB	ASN	21	50.929	16.375	50.212	1.00	83.98
35	169	CG	ASN	21	50.907	15.025	49.599	1.00	83.98
	170	OD1	ASN	21	50.088	14.203	49.969	1.00	83.98
	171 172	ND2 C	ASN ASN	21	51.791	14.775	48.651	1.00	83.98
	173	ŏ	ASN	21 21	49.661 49.706	18.458 19.317	50.598	1.00	82.14
40	174	N	VAL	22	49.715	18.739	49.727 51.889	1.00 1.00	82.14
	175	CA	VAL	22	49.809	20.109	52.347	1.00	82.30 82.30
	176	CB	VAL	22	48.407	20.695	52.489	1.00	52.62
	177	CG1	VAL	22	47.687	19.993	53.637	1.00	52.62
45	178 179	CG2 C	VAL VAL	22 22	48.473	22.229	52.679	1.00	52.62
	180	ŏ	VAL	22	50.502 50.248	20.090 19.192	53.698	1.00	82.30
	181	Ň	THR	23	51.376	21.063	54.503 53.9 5 4	1.00 1.00	82.30 73.57
	182	CA	THR	23	52.083	21.109	55.231	1.00	73.57 73.57
50	183	CB	THR	23	53.598	21.205	55.035	1.00	78.82
50	184	OG1	THR .	23	54.021	20.223	54.076	1.00	78.82
	185 186	CG2 C	THR THR	23	54.309	20.974	56.380	1.00	78.82
	187	ŏ	THR	23 23	51.658 51.640	22.281	56.097	1.00	73.57
	188	Ň	LEU	24	51.549 51.417	23.407 22.007	55.618 57.374	1.00 1.00	73.57
55	189	CA	LEU	24	51.026	23.040	58.314	1.00	80.82 80.82
	190	CB	LEU	24	49.818	22.605	59.138	1.00	72.07
	191	CG	LEU	24	18.578	22.217	58.346	1.00	72.07
	192 193	CD1 CD2	LEU	24	47.353	22.285	59.242	1.00	72.07
60	194	· C	LEU	24 24	48.412 52.188	23.157 23.322	57.182	1.00	72.07
	195	ŏ	LEU	24	52.771	22.420	59.239 59.825	1.00 1.00	80.82
	196	N	THR	25	52.527	24.591	59.367	1.00	80.82 57.44
	197	CA	THR	25	53.622	24.995	60.228	1.00	57.44
65	198	CB	THR	25	54.748	25.593	59.431	1.00	58.08
O)	199 200	OG1 CG2	THR	25	55.299	24.593	58.568	1.00	58.08
	201	C	THR THR	25 25	55.812 53.107	26.103	60.372	1.00	58.08
	202	ŏ	THR	25 25	53.197 52.524	26.039 27.007	61.238	1.00	57.44
-	203	N	CYS	26	53.589	27.007 25.833	60.891 62.489	1.00 1.00	57.44 94.33
70	204	CA	CYS	26	53.276	26.780	63.551	1.00	94.33 94.33
									- 1.00

	205 206	C	CYS	26 ⁻	54.464	27.725	63.557	1.00	94.33
	207	O CB	CYS CYS	26 26	55.604 53.206	27.267 26.060	63.459 64.890	1.00	94.33
	208	SG	CYS	26	52.191	26.860	66.176	1.00 1.00	89.97
5	209	N	ASN	27	54.229	29.031	63.651	1.00	89.97 88.38
	210	CA	ASN	27	55.363	29.941	63.665	1.00	88.38
	211 212	CB CG	ASN ASN	27	55.584	30.555	62.273	1.00	163.21
	213	OD1	ASN	27 27	56.225 57.082	29.574 28.768	61.290 61.667	1.00	163.21
10	214	ND2	ASN	27	55.825	29.654	60.020	1.00 1.00	163.21 163.21
	215	С	ASN	27	55.336	31.039	64.719	1.00	88.38
	216	0	ASN	27	54.563	31.989	64.641	1.00	88.38
	217 218	N CA	GLY GLY	28 28	56.164	30.862	65.736	1.00	157.55
15	219	C	GLY	28	56.306 57.695	31.863 32.269	66.769 66.353	1.00 1.00	157.55
	220	ŏ	GLY	28	58.644	31.591	66.702	1.00	157.55 157.55
	221	N	ASN	29	57.813	33.337	65.572	1.00	155.07
	222	CA	ASN	29	59.110	33.779	65.057	1.00	155.07
20	223 224	CB CG	ASN ASN	29 29	59.054 57.897	35.252 35.564	64.655	1.00	162.85
20	225	OD1	ASN	29	57.735	34.939	63.723 62.672	1.00 1.00	162.85
	226	ND2	ASN	29	57.088	36.545	64.103	1.00	162.85 162.85
	227	Ç	ASN	29	60.312	33.547	65.963	1.00	155.07
25	228 229	O N	ASN	29	61.386	33.183	65.471	1.00	155.07
23	230	CA	ASN ASN	30 30	60.152 61.241	33.787 33.545	67.269 68.220	1.00	156.06
	231	CB	ASN	30	60.696	33.490	69.653	1.00 1.00	156.06 177.59
	232	CG	ASN	30	60.720	34.850	70.334	1.00	177.59
30	233	OD1	ASN	30	61.733	35.550	70.290	1.00	177.59
30	234 235	ND2 C	ASN ASN	30 30	59.613	35.227	70.970	1.00	177.59
	236	ŏ	ASN	30	61.697 62.886	32.182 31.932	. 67.729 67.477	1.00 1.00	156.06
	237	N	PHE	31	60.702	31.316	67.577	1.00	156.06 152.23
25	238	CA	PHE	31	60.896	30.010	66.990	1.00	152.23
35	239	CB	PHE	31	61.081	30.267	65.497	1.00	158.06
	240 241	CG CD1	PHE PHE	31 31	60.650 59.315	29.154 28.746	64.612	1.00	158.06
	242	CD2	PHE	31	61.573	28.561	64.550 63.769	1.00 1.00	158.06 158.06
40	243	CE1	PHE	31	58.924	27.755	63.653	1.00	158.06
40	244	CE2	PHE	31	61.197	27.579	62.877	1.00	158.06
	245 246	CZ C	PHE PHE	31 31	59.869	27.173	62.810	1.00	158.06
	247	ŏ	PHE	31	62.099 62.836	29.281 28.610	67.576 66.857	1.00 1.00	152.23 152.23
	248	N	PHE	32	62.304	29.414	68.880	1.00	168.63
45	249	CA	PHE	32	63.432	28.752	69.510	1.00	166.63
	250 251	CB CG	PHE	32	63.802	29.479	70.792	1.00	178.95
	252	CD1	PHE PHE	32 32	64.123 63.361	30.923 31.922	70.567 71.164	1.00	178.95
	253	CD2	PHE	32	65.174	31.288	69.723	1.00 1.00	178.95 178.95
50	254	ÇE1	PHE	32	63.631	33.271	70.914	1.00	178.95
	255	CE2	PHE	32	65.452	32.634	69.466	1.00	178.95
	256 257	CZ C	PHE PHE	32 32	64.681	33.629	70.068	1.00	178.95
	258	ŏ	PHE	32 32	63.116 63.884	27.288 26.567	69.760 70.399	1.00 1.00	166.63
55	259	N	GLU	33	61.968	26.864	69.239	1.00	166.63 156.85
	260	ÇA	GLU	33	61.527	25.475	69.315	1.00	156.85
	261 262	CB	GLU	33	62.558	24.582	68.620	1.00	168.05
	263	CD	GLU GLU	33 33	63.153 64.130	25.157 24.188	67.330	1.00	168.05
60	264	OE1	GLU	33	64.854	23.526	66.704 67.477	1.00 1.00	168.05 168.05
	265	OE2	GLU	33	64.175	24.084	65.461	1.00	168.05
	266	C	GLU	33	61.233	24.913	70.708	1.00	156.85
	267 268	O N	GLU VAL	33	60.369	24.046	70.851	1.00	156.85
65	269	CA	VAL	34 34	61.963 61.748	25.376 24.926	71.719 73.095	1.00 1.00	106.92
	270	CB	VAL	34	60.953	25.998	73.882	1.00	106.92 129.93
	271	CG1	VAL	34	60.864	25.626	75.361	1.00	129.93
	272	CG2	VAL	34	61.607	27.359	73.695	1.00	129.93
70	273 274	c o	VAL VAL	34 34	61.011 59.825	23.573 23.521	73.211 73.562	1.00	106.92
-		-	V - No	•	النكون	24.JE	73.302	1.00	106.92

	275	N	SER	35	61.712	22.490	72.883	1.00	178.50
	276	CA	SER	35	61.170	21.135	72.978		
	277	CB:	SER					1.00	178.50
				35	60.683	20.879	74.409	1.00	177.04
_	278	og '	SER	· 35	61.781	20.767	75.302	1.00	177.04
5	279	С	SER	35	60.102	20.645	71.988	1.00	178.50
	280	0	SER	35	60,449	20.069	70.956	1.00	178.50
	281	N	SER	36	58.816	20.858	72.286	1.00	
	282	CA	SER	36		20.347			97.16
					57.742		71.411	1.00	97.16
10	283	CB	SER	36	57.175	19.038	71.993	1.00	145.01
10	284	QG	SER	36	58.160	18.018	72.059	1.00	145.01
	285	C	SER	36	56.560	21.259	71.061	1.00	97.16
	286	0	SER	36	56.405	22,357	71.604	1.00	
	287	N	THR	37	55.725	20.750			97.16
							70.149	1.00	111.12
15	288	CA	THR	37	54.530	21. 43 3	69.638	1.00	111.12
15	289	CB	THR	37	54.686	21.780	68.144	1.00	142.34
	290	OG1	THR	37	55.863	22.572	67.954	1.00	142.34
	291	CG2	THR	37	53.465	22.536	67.638	1.00	
	292	Č	THR	37	53.273	20.565			142.34
	293						69.746	1.00	111.12
20		0	THR	37	53.323	19.357	69.509	1.00	111.12
20	294	N	LYS	38	52.147	21.193	70.075	1.00	89.74
	295	CA	LYS	38	50.879	20.480	70.195	1.00	89.74
	296	CB	LYS	38	50.253	20.739	71.559	1.00	
	297	CG	LYS	38	50.833	19.880			101.72
							72.648	1.00	101.72
25	298	CD	LYS	38	50.223	20,211	73.991	1.00	101.72
25	299	CE	LYS	38	50.893	19.410	75.110	1.00	101.72
	300	NZ	LYS	38	50.571	19.965	76.465	1.00	101.72
	301	С	LYS	38	49.889	20.878	69.112	1.00	89.74
	302	ŏ	LYS	38	49.478	22.036			
	303						69.039	1.00	89.74
30		N	TRP	39	49.501	19,911	68.280	1.00	92.70
JU	304	CA	TRP	39	48.549	20.162	67.196	1.00	92.70
	305	CB	TRP	39	48.948	19.417	65.933	1.00	89.95
	306	CG	TRP	39	50.148	19.958	65.279	1.00	89.95
	307	CD2	TRP	39	50.188	21.016	64.329	1.00	
	308	CE2	TRP	39				1.00	89.95
35					51.536	21.192	63.941	1.00	89.95
33	309	CE3	TRP	39	49.211	21.846	63.759	1.00	89.95
	310	CD1	TRP	39	51.438	19.535	65.441	1.00	89.95
	311	NE1	TRP	39	52.282	20.269	64.639	1.00	89.95
	312	CZ2	TRP	39	51.938	22.145	63.017	1.00	89.95
	313	CZ3	TRP	39	49.603	22.799	62.839	1.00	
40	314	CH2	TRP	39					89.95
70					50.958	22.943	62.475	1.00	89.95
	315	Č	TRP	39	47.139	19.743	67.541	1.00	92.70
	316	0	TRP	39	46.926	18.717	68.177	1.00	92.70
	317	N	PHE	40	46.167	20.522	67.096	1.00	74.21
	318	CA	PHE	40	44.782	20.188	67.382	1.00	74.21
45	319	CB	PHE	40	44,177	21.186			
	320	CG					68.365	1.00	91.61
			PHE	40	44.868	21.229	69.698	1.00	91.61
	321	CD1	PHE	40	46.143	21.793	69.829	1.00	91.61
	322	CD2	PHE	40	44.231	20.730	70.833	1.00	91.61
	323	CE1	PHE	40	46.761	21.876	71.069	1.00	91.61
50	324	CE2	PHE	10	44.839	20.807	72.078	1.00	
	325	cz	PHE						91.61
				40	46.110	21.379	72.196	1.00	91.61
	326	C	PHE	40	43.946	20.149	66.121	1.00	74.21
	327	0	PHE	40	43.709	21.176	65.474	1.00	74.21
	328	N	HIS	41	43.506	18.948	65.774	1.00	72.61
55	329	CA	HIS	41	42.691	18.750	64.593	1.00	72.61
	330	CB	HIS	41	43.15C	17.481			
							63.880	1.00	96.01
	331	CG	HIS	41	42.346	17.151	62.661	1.00	96.01
	332	CD2	HIS	41	42.300	16.023	61.911	1.00	96.01
	333	ND1	HIS	.41	41.489	18.048	62.073	1.00	96.01
60	334	CE1	HIS	41	40.942	17.489	61.005	1.00	96.01
	335	NE2	HIS	41	41.419	16.264			
	336	C	HIS				60.887	1.00	96.01
				41	41.223	18.646	64.999	1.00	72.61
	337	0	HIS	41	40.831	17.703	65.696	1.00	72.61
15	338	Ŋ	ASN	42	40.419	19.616	64.563	1.00	65.96
65	339	CA	ASN	42	38.998	19.638	64.896	1.00	65.96
	340	C8	ASN	42	38.304	18.373	64.347	1.00	107.42
	341	œ	ASN	42	37.832	18.533			
	342	OD1	ASN				62.897	1.00	107.42
				42	38.115	19.550	62.262	1.00	107.42
70	343	ND2	ASN	42	37.110	17.532	62.380	1.00	107.42
70	344	С	ASN	42	38.869	19.713	66.422	1.00	65.96
				•					30.03
						•			

	345	0	ASN	42 ·	37.863	19.297	67.008	1.00	65.96
	346	N	GLY	43	39.916	20.229	67.058	1.00	142.69
	347	CA:	GLY	43	39.930	20.362	68.505	1.00	142.69
5	348 349	C	GLY GLY	43 43	40.418	19.152	69.292	1.00	142.69
,	350	N	SER	43 44	40.304 40.972	19.125 18.149	70.508	1.00	142.69
	351	ĊA	SER	44	41.448	16.960	68.621 69.318	1.00 1.00	82.57
	352	СВ	SER	44	40.876	15.716	68.658	1.00	82.57 65.56
	353	OG	SER	44	41.042	14.585	69.496	1.00	65.56
10	354	C	SER	44	42.966	16.877	69.294	1.00	82.57
	355	0	SER	44	43.558	16.765	68.218	1.00	82.57
	356 357	N CA	LEU LEU	45	43.601	16.910	70.464	1.00	83.34
	357 358	CB	LEU	45 45	45.056 45.586	16.846 16.632	70.490	1.00	83.34
15	359	CG	LEU	45	47.121	16.657	71.930 72.177	1.00 1.00	79.17
	360	CD1	LEU	45	47.758	17.921	71.590	1.00	79.17 79.17
	361	CD2	LEU	45	47.403	16.581	73.681	1.00	79.17
	362	C	LEU	45	45.537	15.736	69.542	1.00	83.34
20	363 364	0 N	LEU	45	45.074	14.588	69.585	1.00	83.34
20	365	CA	SER SER	46 46	46.447	16.125	68.658	1.00	133.67
	366	CB	SER	46	47.037 47.551	15.236 16.059	67.671 66.487	1.00	133.67
	367	ÖĞ	SER	46	48.435	15.315	65.662	1.00 1.00	75.61 75.61
	368	C	SER	46	48.196	14.486	68.299	1.00	133.67
25	369	0	SER	46	48.864	15.000	69.195	1.00	133.67
	370	N	GLU	47	48.431	13.268	67.827	1.00	113.73
	371 372	CA CB	GLU	47	49.545	12.470	68.329	1.00	113.73
	372 373	CG	GLU	47 47	49.354	10.985	67.982	1.00	165.00
30	374	CD	GLU	47	48.217 48.093	10.318 8.817	68.775 68.530	1.00	165.00
	375	OE1	GLU	47	47.813	8.412	67.380	1.00 1.00	165.00 165.00
	376	OE2	GLU	47	48.270	8.039	69.494	1.00	165.00
	377	C	GLU	47	50.821	13.023	67.695	1.00	113.73
35	378	O N	GLU	47	51.921	12.506	67.908	1.00	113.73
33	379 380	ČA	GLU	48 48	50.650	14.089	66.915	1.00	132.93
	381	CB	GLU	48	51. 755 51. 26 4	14. 763 15.424	66.249 64.9 6 6	1.00	132.93
	382	CG	GLU	48	52.348	16.113	64.173	1.00 1.00	192.46 192.46
	383	CD	GLU	48	52.450	15.579	62.762	1.00	192.46
40	384	OE1	GLU	48	51.665	14.672	62.406	1.00	192.46
	385	OE2	GLU	48	53.316	16.062	62.005	1.00	192.46
	386 387	CO	GLU	48 48	52.280	15.826	67.207	1.00	132.93
	388	Ň	THR	40 49	51. 506 53. 5 91	16.635 15.827	67.730 67.436	1.00 1.00	132.93
45	389	CA	THR	49	54.193	16.789	68.350	1.00	120.56 120.56
	390	CB	THR	49	54.823	16.075	69.569	1.00	154.93
	391	OG1	THR	49	55.638	14.984	69.123	1.00	154.93
	392	CG2	THR	49	53.740	15.552	70.504	1.00	154.93
50	393 394	C	THR THR	49	55.248	17.684	67.713	1.00	120.56
50	395	N	ASN	49 50	55. 697 55. 639	18.652 17.368	68.323	1.00	120.56
	396	CA	ASN	50	56.646	18.154	66.484 65.779	1.00 1.00	120.79
	397	CB	ASN	50	57.190	17.349	64.596	1.00	120.79 183.19
EE	398	CG	ASN	50	57.793	16.024	65.035	1.00	183.19
55	399	OD1	ASN	50	58.218	15.900	66.182	1.00	183.19
	400 401	ND2 C	ASN	50	57.865	15.054	64.124	1.00	183.19
	402	ŏ	ASN ASN	50 50	56.070 54.854	19.485 19.616	65.312 65.460	1.00	120.79
	403	Ň	SER	51	56.944	20.466	65.160 65.084	1.00 1.00	120.79 104.18
60	404	CA	SER	51	56.522	21.811	64.657	1.00	104.18
	405	CB	SER	51	57. 73 5	22.751	64.577	1.00	100.13
	406	OG	SER	51	58. 55 9	22.431	63.468	1.00	100.13
	407 408	C	SER	51	55.753	21.880	63.329	1.00	104.18
65	408 409	0 N	SER SER	51 52	55.086 55.086	22.879	63.053	1.00	104.18
05	410	CA	SER	52 52	55.858 55.154	20.835 20.803	62.507	1.00	108.20
	411	CB	SER	52	56.131	20.860	61.223 60.041	1.00 1.00	108.20 83.34
	412	OG	SER	52	56.705	22.151	59.913	1.00	83.34 83.34
70	413	C	SER	52	54.291	19.566	61.083	1.00	108.20
70	414	0	SER	52	54.750	18.445	61.284	1.00	108.20

	415 416	N CA	LEU	53 ⁻ 53	53.038 52.057	19.790 18.730	60.720	1.00	62.72
	417	CB.	LEU	53	50.730	19.214	60.536 61.130	1.00	62.72
	418	CG	LEU	53	49.456	18.379	61.050	1.00 1.00	43.93
5	419	CD1	LEU	53	49.665	17.079	61.786	1.00	43.93 43.93
	420	CD2	LEU	53	48.305	19.148	61.680	1.00	43.93
	421	Ç	LEU	53	51.912	18.398	59.035	1.00	62.72
	422	0	LEU	53	51.470	19.226	58.234	1.00	62.72
10	423 424	N	ASN	54	52.294	17.192	58.642	1.00	92.98
10	425	CA CB	ASN ASN	54 54	52.183	16.832	57.236	1.00	92.98
	426	ČĠ	ASN	54 54	53.404 54.670	16.036 16.844	56. 796	1.00	86.69
	427	OD1	ASN	54	54.805	17.866	56. 872 56.1 8 6	1.00 1.00	86.69
	428	ND2	ASN	54	55.608	16.406	57.717	1.00	86.69
15	429	С	ASN	54	50.941	16.029	56.929	1.00	86.69 92.98
	430	0	ASN	54	50.701	14.991	57.529	1.00	92.98
	431	N	ILE	55	50.144	16.523	55.995	1.00	45.24
	432	CA	ILE	55	48.935	15.823	55.582	1.00	45.24
20	433 434	CB CG2	ILE	55 55	47.716	16.773	55.491	1.00	31.24
20	435	CG1	ILE	55 55	46.623 47.183	∶5.157 17.072	54.647	1.00	31.24
	436	CD1	ILE	55	45.969	17.961	56. 884 56.867	1.00	31.24
	437	Č.	ILE	55	49.224	15.251	54.200	1.00 1.00	31.24
	438	Ó	ILE	55	49.262	15.977	53.201	1.00	45.24 45.24
25	439	N	VAL	56	49.437	13.942	54.160	1.00	82.87
	440	CA	VAL.	56	49.730	13.244	52.923	1.00	82.87
	441	CB	VAL	56	50.831	. 12.192	53.155	1.00	72.67
	442 443	CG1	VAL	56	51.176	11.489	51.856	1.00	72.67
30	444	CG2 C	VAL VAL	56 50	52.057	12.862	53.731	1.00	72.67
50	445	ŏ	VAL	56 56	48.467 47.689	12.569 12.010	52.398	1.00	82.87
	446	Ň	ASN	57	48.268	12.636	53.171 51.085	1.00 1.00	82.87
	447	CA	ASN	57	47.099	12.059	50.438	1.00	59.63 59.63
~~	448	CB	ASN	57	47.302	10.562	50.308	1.00	98.65
35	449	CG	ASN	57	48.632	10.237	49.655	1.00	98.65
	450	OD1	ASN	57	48.980	10.808	48.609	1.00	98.65
	451 452	ND2	ASN	57	49.391	9.331	50.267	1.00	98.65
	452 453	C	ASN ASN	57	45.864	12.412	51.249	1.00	59.63
40	454	Ň	ALA	57 58	45.322 45.443	11.593 13.665	51.998	1.00	59.63
	455	CA	ALA	58	44.300	14.216	51.090 51.809	1.00 1.00	71.80
	456	CB	ALA	58	43.991	15.617	51.310	1.00	71.80 87.99
	457	С	ALA	58	43.073	13.358	51.690	1.00	71.80
45	458	0	ALA	58	42.783	12.818	50.625	1.00	71.80
45	459	N _.	LYS	59	42.363	13.240	52.805	1.00	72.92
	460	CA	LYS	59	41.128	12.467	52.885	1.00	72.92
	461 462	CB CG	LYS	59 50	41.293	11.281	53.830	1.00	124.59
	463	CD	LYS LYS	59 59	42.422 42.480	10.361	53.457	1.00	124.59
50	464	CE	LYS	5 9	43.356	9.187 8.128	54.387 53.783	1.00	124.59
	465	NZ	LYS	59	43.282	6.869	54.581	1.00 1.00	124.59
	466	C	LYS	59	40.082	13.397	53.457	1.00	124.59 72.92
	467	0	LYS	59	40.356	14.132	54.401	1.00	72.92
<i>E E</i>	468	N	PHE	60	38.887	13.381	52.897	1.00	56.87
55	469	CA	PHE	60	37.848	14.255	53.416	1.00	56.87
	470 471	CB	PHE	60	36.488	13.707	53.028	1.00	109.01
	472	CG CD1	PHE	60	36.292	13.613	51.562	1.00	109.01
	473	CD2	PHE	60 60	35.499	12.629	51.015	1.00	109.01
60	474	CE1	PHE	60	36.957 35.336	14.485 12.536	50.714	1.00 1.00	109.01
	475	CE2	PHE	60	36.803	14.404	49.634 49.337	1.00	109.01 109.01
	476	CZ	PHE	60	36.006	13.414	48.793	1.00	109.01
	477	C	PHE	60	37.930	14.414	54.928	1.00	56.87
C E	478	0	PHE	60	37.628	15.478	55.475	1.00	56.87
65	479	N	GLU	61	38.352	13.350	55.598	1.00	64.50
	480	CA	GLU	61	38.460	13.336	57.054	1.00	64.50
	481 482	CB CG	GLU	61	38.892	11.953	57.542	1.00	154.96
	483	CD	GLU	61 61	37.855	10.870	57.334	1.00	154.96
70	484	OE1	GLU	61	37.517 38.443	10.655 10.355	55.871 55.097	1.00	154.96
	-	32.		•	JU. 770	10.000	55.087	1.00	154.96

	485	OE2	GLU	61 ⁻	36.328	10.784	55.505	1.00	154.00
	486	С	GLU	61	39.436	14.356	57.576	1.00	154.96 64.50
	487	0	GLU	61	39.351	14.765	58.731	1.00	64.50
_	488	N	ASP	62	40.371	14.745	56.713	1.00	71.49
5	489	CA	ASP	62	41.404	15.723	57.035	1.00	71.49
	490	CB	ASP	62	42.574	15.543	56.079	1.00	78.68
	491	CG	ASP	62	43.412	14.316	56.422	1.00	78.68
	492	OD1	ASP	62	43.641	14.093	57.639	1.00	78.68
10	493	OD2	ASP	62	43.851	13.594	55.485	1.00	78.68
10	494	С	ASP	62	40.883	17.160	57.000	1.00	71.49
	495	0	ASP	62	41.574	18.102	57.400	1.00	71.49
	496	N	SER	63	39.654	17.326	56.523	1.00	52.56
	497	CA	SER	63	39.056	18.637	56.490	1.00	52.56
15	498	CB	SER	63	37.722	18.586	55.773	1.00	54.10
13	499	og	SER	63	37.914	18.110	54.456	1.00	54.10
	500	C	SER	63	38.850	19.020	57.936	1.00	52.56
	501 502	O N	SER	63	39.035	18.202	58.826	1.00	52.56
	503	CA	GLY GLY	64	38.479	20.268	58.171	1.00	71.62
20	504	c	GLY	64	38.243	20.690	59.528	1.00	71.62
20	505	ŏ	GLY	64	39.138	21.809	59.962	1.00	71.62
	506	Ň	GLU	64 65	39.954	22.299	59.196	1.00	71.62
	507	CA	GLU	65	38.957 39.712	22.205	61.211	1.00	87.67
	508	CB	GLU	65	38.887	23.270	61.833	1.00	87.67
25	509	CG	GLU	65	39.602	23.868	62.967	1.00	86.11
	510	CD	GLU	65	38.934	24.889 25.056	63.834	1.00	86.11
	511	OE1	GLU	65	39.124	24.172	65.194	1.00	86.11
	512	OE2	GLU	65	38.210	26.059	66.068 65.386	1.00 1.00	86.11
	513	C	GLU	65	40.988	22.684	62.395	1.00	86.11
30	514	Ö	GLU	65	41.072	21.485	62.640	1.00	87.67 87.67
	515	N	TYR	66	41.980	23.539	62.598	1.00	99.15
	516	CA	TYR	66	43.258	23.129	63.151	1.00	99.15
	517	CB	TYR	66	44.246	22.786	62.044	1.00	44.24
0.5	518	CG	TYR	66	44.017	21.547	61.224	1.00	44.24
35	519	CD1	TYR	66	43.042	21,512	60.225	1.00	44.24
	520	CE1	TYR	66	42.884	20.381	59.401	1.00	44.24
	521	CD2	TYR	66	44.838	20.429	61.399	1.00	44.24
	522	CE2	TYR	66	44.700	19.299	60.600	1.00	44.24
40	523	CZ	TYR	66	43.719	19.270	59. 59 6	1.00	44.24
40	524 525	он	TYR	66	43.560	18.121	58. 82 2	1.00	44.24
	525 526	C	TYR	66	43.848	24.303	63.935	1.00	99.15
	526 527	O N	TYR LYS	66	43.714	25.462	63.526	1.00	99.15
	528	CA	LYS	67 67	44.502	' 23.996	65.052	1.00	76.23
45	529	CB	LYS	67 67	45.158	25.008	65.883	1.00	76.23
	530	CG	LYS	67	44.357 42.934	25.311 25.780	67.152	1.00	84.41
	531	CD	LYS	67	42.212	25.802	66.944 68.294	1.00	84.41
	532	CE	LYS	67	40.725	26.104	68.164	1.00	84.41
	533	NZ	LYS	67	40.042	25.844	69.456	1.00 1.00	84.41
50	534	C	LYS	67	46.477	24.393	66.303	1.00	84.41 76.23
	535	0	LYS	67	46.621	23.170	66.300	1.00	76.23
	538	N	CYS	68	47.449	25.235	66.825	1.00	101.62
	537	CA	CYS	68	48.729	24.757	67.110	1.00	101.62
	538	С	CYS	68	49.018	25.644	68.203	1.00	101.62
55	539	0	CYS	68	48.586	26. 79 7	68.355	1.00	101.62
	540	CB	CYS	68	49.836	24.883	66.058	1.00	149.58
	541	SG	CYS	68	50.287	26.560	65.501	1.00	149.58
	542	N.	GLN	69	49.716	25.099	69.281	1.00	93.84
60	543	CA	GLN	69	50.045	25.874	70.458	1.00	93.84
w	544	CB	GLN	69	48.935	25.756	71.497	1.00	108.47
	545 546	CG	GLN	69	49.325	26.336	72.838	1.00	108.47
	547	CD OE1	GLN	69	48.228	26.198	73.866	1.00	108.47
	547 548	NE2	GLN	69	47.421	25.266	73.801	1.00	108.47
65	549	NE2 C	GLN GLN	69	48.197	27.116	74.835	1.00	108.47
	550	ŏ	GLN	69 60	51.362	25.450	71.087	1.00	93.84
	551	Ň	HIS	69 70	51.813	24.310	70.919	1.00	93.84
	552	ČA	HIS	70 70	51.986 53.221	26.399 26.162	71.778	1.00	149.64
	553	CB	HIS	70	54.272	26.162 27.216	72.504 72.161	1.00	149.64
70	554	čĠ	HIS	70 70	54.952	26.965	72.161 70.957	1.00	188.52
		- -	•		J-1.00E	20.000	70.857	1.00	168.52

	555	CD2	HIS	70 ·	54.804	25.981	69.844	1.00	188.52
	556	ND1	HIS	. 70	55.951	27.788	70.358	1.00	188.52
	557	CE1	HIS	70	56.375	27.316	69.210	1.00	188.52
5	558	NE2	HIS	70	55.693	26.212	68.928	1.00	188.52
5	559 560	C	HIS HIS	70	52.788	26.284	73.952	1.00	149.64
	561	N	GLN	70 71	52.566 52.642	27.385 25.132	74.454	1.00	149.64
	562	CA	GLN	71	52.042 52.191	25.132 25.045	74.599 75.981	1.00	126.80
	563	СВ	GLN	71	52.974	23.964	76. 72 6	1.00 1.00	126.80
10	564	CG	GLN	71	52.367	23.589	78.072	1.00	175.94 175.94
	565	CD	GLN	71	53.119	22.461	78.752	1.00	175.94
	566	OE1	GLN	71	54.130	21.984	78.241	1.00	175.94
	567 568	NE2	GLN	71	52.631	22.031	79.909	1.00	175.94
15	569	C O	GLN GLN	71 71	52.267	26.359	76.745	1.00	126.80
13	570	Ň	GLN	71 72	53.343 51.096	26.934 26.825	76.927	1.00	126.80
	571	CA	GLN	72	50.936	28.060	77.169 77.933	1.00 1.00	138.09
	572	СВ	GLN	72	51.762	28.017	79.214	1.00	138.09 197.82
20	573	CG	GLN	72	51.264	27.031	80.242	1.00	197.82
20	574	CD	GLN	72	49.767	27.138	80.538	1.00	197.82
	575 5 76	OE1 NE2	GLN	72	49.158	28.202	80.397	1.00	197.82
	577	C	GLN GLN	72 72	49.175	26.028	80.973	1.00	197.82
	578	ŏ	GLN	72 72	51.252 51.503	29.347 30.377	77.196	1.00	138.09
25	579	Ň	VAL	73	51.243	29.291	77.821 75.871	1.00	138.09
	580	CA	VAL	73	51.505	30.477	75.070	1.00 1.00	127.03
	581	CB	VAL	73	52.817	30.340	74.250	1.00	127.03 90.79
	582	CG1	VAL	73	53.197	31.683	73.626	1.00	90.79
30	583	CG2	VAL	73	53.943	29.826	75.148	1.00	90.79
30	584 585	C	VAL VAL	73	50.314	30.625	74.134	1.00	127.03
	586	N	ASN	73 74	50.467 49.119	30.866	72.936	1.00	127.03
	587	ĊA	ASN	74	47.890	30.457 30.577	74.693 73.920	1.00	129.72
	588	СВ	ASN	74	47.721	31.993	73.390	1.00 1.00	129.72 137.31
35	589	CG	ASN	74	47.576	33.011	74.476	1.00	137.31
	590	OD1	ASN	74	48.512	33.785	74.713	1.00	137.31
	591 592	ND2	ASN	74	46.400	33.015	75.123	1.00	137.31
	593	C	ASN ASN	74 74	47.820	29.655	72.709	1.00	129.72
40	594	Ň	GLU	7 4 75	48.836 46.600	29.209 29.404	72.176 72.254	1.00	129.72
	595	CA	GLU	75	46.377	28.580	71.080	1.00 1.00	128.29 128.29
	5 9 6	CB	GLU	.75	44.998	27.934	71.175	1.00	132.07
	597	CG	GLU	75	44.672	27.459	72.584	1.00	132.07
45	598	CD	GLU	75	43.266	26.922	72.700	1.00	132.07
40	599 600	OE1 OE2	GLU GLU	75	42.439	27.252	71.821	1.00	132.07
	601	C	GLU	75 75	42.989	26.185	73.673	1.00	132.07
	602	ŏ	GLU	75 75	46.446 48.432	29.547 30.757	69.897 70.089	1.00	128,29
	603	N	SER	76	48.545	29.033	68.681	1.00 1.00	128.29 77,19
50	604	CA	SER	76	46.595	29.901	67.506	1.00	77.19 77.19
	605	CB	SER	76	47.321	29.207	66.363	1.00	54.46
	606	og	SER	76	46.418	28.351	65.649	1.00	54.46
	607 608	C	SER	76	45.175	30.169	67.033	1.00	77.19
55 ·	609	O N	SER GLU	76 77	44.208 45.038	29.659	67.603	1.00	77.19
	610	CA	GLU	77	43.711	30.966 31.198	65.983 65.444	1.00	74.40
	611	CB	GLU	77	43.652	32.492	64.632	1.00 1.00	74.40 153.94
	612	CG	GLU	77	43.693	33.746	65.491	1.00	153.94
۲۸	613	CD	GLU	77	42.624	33.749	66.578	1.00	153.94
60	614	OE1	GLU	77	41.418	33.712	66.237	1.00	153.94
	615 616	OE2 C	GLU	77	42.992	33.787	67.775	1.00	153.94
	617	ŏ	GLU GLU	77 77	43.460	29.998	64.558	1.00	74.40
	618	Ň	PRO	77 78	44.375 42.215	29.495 29.512	63.913 84.527	1.00	74.40
65	619	CD	PRO	78	41.068	29.938	64.527 65.344	1.00 1.00	88.95 122.79
	620	CA	PRO	78	41.857	28.352	63.712	1.00	88.95
	621	CB	PRO	78	40.385	28.138	64.046	1.00	122.79
	622	ça	PRO	78	40.268	28.670	65.428	1.00	122.79
70	623 624	CO	PRO	78 70	42.061	28.542	62.221	1.00	88.95
. •	· 7	•	PRO	78	41.901	29.640	61.688	1.00	88.95

	625	N	VAL	79 .	42.415	27.447	61.560	1.00	101.07
	626	CA	VAL	79	42.604	27.427	60.119	1.00	101.27 101.27
	627	CB	VAL	79	44.042	27.114	59.735	1.00	79.48
Š	628 629	CG1 CG2	VAL VAL	79 79	44.177	27.097	58.226	1.00	79.48
,	630	C	VAL	79 79	44.962 41.727	28.130 26.304	60.341 59.592	1.00 1.00	79.48
	631	Ö	VAL	79	41.846	25.155	60.025	1.00	101 <i>.2</i> 7 101.27
	632	N	TYR	80	40.851	26.629	58.655	1.00	55.37
10	633	CA	TYR	80	39.973	25.618	58.115	1.00	55.37
10	634 635	CB CG	TYR TYR	80 80	38.551 38.004	26.145 26.497	58.016 50.264	1.00	122.28
	636	CD1	TYR	80	38.278	27.733	59.364 59.942	1.00 1.00	122.28 122.28
	637	CE1	TYR	80	37.817	28.049	61.208	1.00	122.28
15	638	CD2	TYR	80	37.250	25.577	60.088	1.00	122.28
13	639 640	CE2 CZ	TYR TYR	80 80	36.782	25.877 27.117	61.357	1.00	122.28
	641	OH	TYR	80	37.069 36.615	27.117 27.424	61.915 63.180	1.00 1.00	122.28 122.28
	642	C	TYR	80	40.390	25.066	56.779	1.00	55.37
20	643	0 .	TYR	80	40.474	25.780	55.795	1.00	55.37
20	644 645	N CA	LEU	81	40,627	23.768	56.765	1.00	67.93
	646	CB	LEU	81 81	41.026 42.016	23.065 22.014	55. 578 55.982	1.00 1.00	67.93
	647	CG	LEU	81	42.558	21.223	.54.819	1.00	70.09 70.09
25	648	CD1	LEU	81	43.387	22.150	53.967	1.00	70.09
25	649 CE0	CD2	LEU	81	43.411	20.066	55.338	1.00	70.09
	650 651	C	LEU	81 81	39 79† 38.856	22.405 22.098	55.006 55.760	1.00	67.93
	652	Ň	GLU	82	39.732	22.188	55.763 53.691	1.00 1.00	67.93 70.25
20	653	CA	GLU	82	38.569	21.530	53.079	1.00	70.25
30	654	CB	GLU	82	37.486	22.562	52.737	1.00	131.12
	655 656	CG CD	GLU GLU	82 82	36.199 34.994	21.935 22.847	52.234	1.00	131.12
	657	OE1	GLU	82	35.091	24.023	52.359 51.958	1.00 1.00	131.12 131.12
0.5	658	OE2	GLU	82	33.940	22.384	52.847	1.00	131.12
35	659	C	GLU	82	38.957	20.709	51.843	1.00	70.25
	660 661	O N	GLU VAL	82 83	39.425	21.261	50.850	1.00	70.25
	662	ČA	VAL	83	38. 769 39.106	19.386 18.469	51.918 50.815	1.00 1.00	52.36 52.36
40	663	CB	VAL	83	39.452	17.094	51.350	1.00	43.44
40	664	CG1	VAL	83	40.082	16.245	50.244	1.00	43.44
	665 666	CG2 C	VAL VAL	83 83	40.359	17.241	52.544	1.00	43.44
	667	ŏ	VAL	83	37.995 36.852	18.302 18.022	49.768 50.105	1.00 1.00	52.36 52.36
	668	N	PHE	84	38.342	18.479	48.498	1.00	63.83
45	669	CA	PHE	84	37.368	18.369	47.426	1.00	63.83
	670 671	CB CG	PHE	84 84	37.359	19.633	46.562	1.00	62.38
	672	CD1	PHE	84 84	36.918 37.692	20.841 21.345	47.294 48.329	1.00 1.00	62.38
	673	CD2	PHE	84	35.680	21.429	47.020	1.00	62.38 62.38
50	674	CE1	PHE	84	37.244	22.418	49.092	1.00	62.38
	675 676	CE2 CZ	PHE	84	35.223	22.506	47.780	1.00	62.38
	677	C C	PHE	84 84	36.007 37.606	22.998 17.175	48.823 46.527	1.00	6º 38
	678	ŏ	PHE	84	38.619	16.477	46. 63 0	1.00 1.00	63.83 63.83
55	679	N	SER	85	36.635	16.952	45.650	1.00	70.22
	680	CA	SER	85	38.663	15.891	44.671	1.00	70.22
	681 682	CB CB	SER SER	85 85	36.006 36.099	14.615	45.197	1.00	107.42
	683	č	SER	85	35.833	13.567 16.465	44.235 43.552	1.00 1.00	107.42 70.22
60	684	0	SER	85	34.608	16.501	43.625	1.00	70.22
	685	N	ASP	86	36.513	16.953	42.528	1.00	30.45
	686 687	CA CB	ASP ASP	86 86	35.835 35.151	17.517	41.391	1.00	30.45
	688	CG	ASP	86	35.151 34.005	18. 79 6 19.121	41.799 40.908	1.00 1.00	66.75 66.75
65	689	OD1	ASP	86	34.186	19.182	39.664	1.00	66.75
	690	OD2	ASP	86	32.909	19.311	41.455	1.00	68.75
	691 692	C	ASP ASP	86	36.876	17.768	40.303	1.00	30.45
	693	Ň	TRP	86 87	38.074 36.427	17.603 18.122	40.551 39.101	1.00 1.00	30.45
70	694	CA	TRP	87	37.329	18.392	37.986	1.00	54.88 54.88
							-		JJ

	695	CB	TRP	87	36.541	18.398	36.686	1.00	120.63
	696	CG	TRP	87	36,228	17.051	36.187	1.00	120.63
	697	CD2	TRP	87	35.123	16,242	36.559	1.00	
_	698	CE2	TRP	87	35.205	15.040	35.822	1.00	120.63
5	699	CE3	TRP	87	34.043	16.411	37.446	1.00	120.63
	700	CD1	TRP	87	36.936	16.335	35.269	1.00	120.63
	701	NE1	TRP	87	36.336	15.125	35.036	1.00	120.63
	702	CZ2	TRP	87	34.277	14.011	35.939	1.00	120.63
	703	CZ3	TRP	87	33.109	15.387	37.568	1.00	120.63
10	704	CH2	TRP	87	33.231	14.202	36.813	1.00	120.63
	705	C	TRP	87	38.051	19.726	38.150	1.00	120.63
	706	0	TRP	87	39.248	19.818	37.884	1.00	54.88
	707	N	LEU	88	37.307	20.751	38.578		54.88
	708	CA	LEU	88	37.831	22.113	38.806	1.00	42.94
15	709	CB	LEU	88	37.131	23.157	37.946	1.00	42.94
	710	CG	LEU	88	37.526	23.193	36.485	1.00	57.40
	711	CD1	LEU	88	36.761	24.330	35.822	1.00	57.40
	712	CD2	LEU	88	39.030	23.370	36. 354	1.00	57.40
	713	C	LEU	88	37.671	22.549	40.235	1.00	57.40
20	714	Ö	LEU	88	36.666	22.301		1.00	42.94
	715	N	LEU	89	38.681	23.225	40.870	1.00	42.94
	716	CA	LEU	89	38.667	23.700	40.733	1.00	58.27
	717	CB	LEU	89	39.556	22.835	42.085	1.00	58.27
	718	CG	LEU	89	39.739	23.331	42.951	1.00	5.00
25	719	CD1	LEU	89			44.403	1.00	5.00
	720	CD2	LEU	89	38.371	23.632	45.112	1.00	5.00
	721	C	LEU	89	40.628 39.237	22.281	45.195	1.00	5.00
	722	ŏ	LEU	89		25.082	42.056	1.00	58.27
	723	Ň	LEU	90	40.346	25.279	41.555	1.00	58.27
30	724	ČA	LEU		38.486	26.043	42.582	1.00	24.40
50	725	CB	LEU	90 90	38.995	27.407	42.636	1.00	24.40
	726	CG	LEU		37.861	28.425	42.585	1.00	63.96
	727	CD1	LEV	90 90	38.331	29.867	42.711	1.00	63.96
	728	CD2	LEU	90	39.284	30.173	41.570	1.00	63.96
35	729	C	LEU	90	37.134	30.803	42.692	1.00	63.96
-	730	ŏ	LEU	90	39.702	27.535	43.969	1.00	24.40
	731	Ň	GLN	90 91	39.057	27.496	45.000	1.00	24.40
	732	CA	GLN	91 91	41.017 41.721	27.690	43.970	1.00	52.44
	733	CB	GLN	91		27.825	45.234	1.00	52.44
40	734	CG	GLN		43.018	27.058	45.151	1.00	32.27
	735	CD	GLN	91	42.820	25.718	44.534	1.00	32.27
	736	OE1	GLN	91	44.020	24.841	44.727	1.00	32.27
	737	NE2	GLN	91	45.010	24.901	43.957	1.00	32.27
	738	C	GLN	91	43.962	24.016	45.788	1.00	32.27
45	739	ŏ		91	41.981	29.299	45.554	1.00	52.44
43	740	Ň	GLN	91	42.060	30.142	44.657	1.00	52.44
	741		ALA	92	42.075	29.633	46.831	1.00	55.47
	742	CA CB	ALA	92	42.345	31.018	47.175	1.00	55,47
	743	CB	ALA	92	41.076	31.735	47.638	1.00	37.36
50	743 744	Ç ·	ALA	92	43.381	31.100	48.246	1.00	55.47
30	744 745	0	ALA	92	43.384	30.316	49.183	1.00	55.47
		N	SER	93	44.263	32.064	48.077	1.00	51.36
	746	CA	SER	93	45.329	32.345	49.008	1.00	51.36
	747	CB	SER	93	45.997	33.647	48.583	1.00	54.66
55	748	og	SER	93	45.009	34.650	48.346	1.00	54.66
22	749	Ç	SER	93	44.690	32.509	50.378	1.00	51.36
	750	o.	SER	93	45.238	32.104	51.395	1.00	51.36
	751	N	ALA	94	43.521	33.124	50.397	1.00	46.22
	752	· CA	ALA	94	42.822	33.313	51.645	1.00	46.22
60	753	СВ	ALA	94	43.522	34.352	52.496	1.00	74.92
W	754	Č	ALA	94	41.393	33.723	51.340	1.00	46.22
	755	0	ALA	94	41.111	34.357	50.317	1.00	46.22
	756	N	GLU	95	40.489	33.326	52.231	1.00	89.58
	757	CA	GLU	95	39.074	33.605	52.065	1.00	89.58
<i>CE</i>	758	CB	GLU	95	38.283	32.448	52.662	1.00	145.77
65	759	CG	GLU	95	38.549	31.139	51.938	1.00	145.77
	760	CD	GLU	95	37.950	29.953	52.650	1.00	145.77
	761	OE1	GLU	95	38.060	28.826	52.118	1.00	145.77
	762	OE2	GLU	95	37.373	30.145	53.742	1.00	145.77
70	763	С	GLU	95	38.662	34.938	52.678	1.00	89.58
70	764	0	GLU	95	37.661	35.546	52.289	1.00	89.58
				•					08.00

	765 766 767	N CA CB:	VAL VAL VAL	96 [.]	39.453 39.233	35.379 36.643	53.644 54.322	1.00	75.49 75.49
_	768	CG1	VAL	96 96	38.995 38.710	36.436 37.771	55.819 56.480	1.00 1.00	87.57 87.57
5	769 770	CG2	VAL	96	37.847	35.467	56.032	1.00	87.57
	770 771	C	VAL VAL	96 96	40.537 41.578	37.402 37.016	54.128 54.665	1.00 1.00	75.49
	772	N	VAL	97	40.482	38.471	53.345	1.00	75.49 96.50
10	773 774	CA CB	VAL VAL	97 97	41.670	39.254	53.066	1.00	96.50
•	775	CG1	VAL	97	41.929 42.920	39.335 40.443	51.553 51.259	1.00 1.00	66.57 66.57
	776	CG2	VAL	97	42.472	38.004	51.049	1.00	66.57
	777 778	C	VAL VAL	97 97	41.598 40.583	40.665 41.352	53.613 £3.473	1.00	96.50
15	779	N	MET	98	42.693	41.088	4.237	1.00 1.00	96.50 97.55
	780 781	CA CB	MET MET	98	42.784	42.425	₹ 1.799	1.00	97.55
	782	CG	MET	98 98	43.870 43.567	42.482 41.601	55.887 57.108	1.00 1.00	148.78 148.78
20	783	SD	MET	98	44.803	41.635	58.454	1.00	148.78
20	784 785	CE C	MET MET	98 98	45.665 43.098	40.108 ∔3.411	58.182	1.00	148.78
	786	ŏ	MET	98	44.143	43.318	53.682 53.034	1.00 1.00	97.55 97.55
	787	N	GLU	99	42.161	44.329	53.455	1.00	85.18
25	788 789	CA CB	GLU GLU	99 99	42.265 41.565	45.380 46.635	52.450	1.00	85.18
	790	CG	GLU	99	41.620	47.868	52.988 52.109	1.00 1.00	186.55 186.55
	791 792	CD	GLU	99	40.716	48.978	52.629	1.00	186.55
	793	OE1 OE2	GLU	99 99	40.827 39.894	49.337 49.490	53.823 51.839	1.00	186.55
30	794	C	GLU	99	43.724	45.677	52.137	1.00 1.00	186.55 85.18
	795 796	0 N	GLU GLY	99	44.605	45.506	52.990	1.00	85.18
	797	CA	GLY	100 100	43.991 45.362	46.106 46.432	50. 9 09 50. 54 9	1.00 1.00	64.51 64.51
35	798	C	GLY	100	46.371	45.293	50.459	1.00	64.51
33	799 800	0 N	GLY GLN	100 101	47.508 45.987	45.528 44.075	50.054	1.00	64.51
	801	CA	GLN	101	46.896	42.930	50.839 50.742	1.00 1.00	91.02 91.02
	802	CB	GLN	101	46.631	41.933	51.875	1.00	93.41
40	803 804	CG CD	GLN GLN	101 101	47.181 48.671	42.383 42.663	53.207 53.133	1.00 1.00	93.41
	805	OE1	GLN	101	49.117	43.530	52.384	1.00	93.41 93.41
	806 807	NE2	GLN	101	49.448	41.926	53.906	1.00	93.41
	808	C	GLN GLN	101 101	46.716 45.909	42.260 42.712	49.373 48.567	1.00 1.00	91.02 91.02
45	809	N ·	PRO	102	47.484	41.195	49.078	1.00	67.73
	810 811	CD CA	PRO PRO	102	48.769	40.802	49.675	1.00	29.55
	812	CB	PRO	102 102	47.324 48.730	40.547 40.145	47.778 47.432	1.00 1.00	67.73 29.55
50	813	ca	PRO	102	49.248	39.718	48.721	1.00	29.55
30	814 815	C	PRO PRO	102 102	46.398 46.385	39.353 38.564	47.784	1.00	67.73
	816	Ň	LEU	103	45.636	39.227	48.719 46.707	1.00 1.00	67.73 40.45
	817	CA	LEU	103	44.688	38.154	46.552	1.00	40.45
55	818 819	CB CG	LEU LEU	103 103	43.308 42.141	38.743 37.774	46.277 46.464	1.00	52.62
	820	CD1	LEU	103	42.345	36.942	46.464 47.721	1.00 1.00	52.62 52
	821 822	CD2	LEU	103	40.852	38.574	46.533	1.00	52.62
	823	C	LEU	103 103	45.115 45.314	37.227 37.665	45.415 44.280	1.00 1.00	40.45 40.45
60	824	N	PHE	104	45.274	35.945	45.739	1.00	56.34
	825 826	CA CB	PHE PHE	104	45.680	34.942	44.762	1.00	56.34
	827	CG	PHE	104 104	46.898 48.053	34.159 35.016	45.251 45.592	1.00 1.00	133.82 133.82
45	828	CD1	PHE	104	48.298	35.367	46.905	1.00	133.82
65	829 830	CD2 CE1	PHE PHE	104 104	48.870	35.528	44.594	1.00	133.82
	831	CE2	PHE	104	49.344 49.924	36.223 36.389	47.229 44.906	1.00 1.00	133.82 133.82
	832	cz	PHE	104	50.161	36.738	46.224	1.00	133.82
70	833 834	C	PHE PHE	104 104	44.570 43.923	33.958 33.468	44.477	1.00	56.34
	•	•		104	43.923	33.468	45.388	1.00	56.34

	835	N	LEU	105	44.363	33.668	43.202	1.00	54.04
	836	CA	LEU	105	43.341	32.730	42.792	1.00	51.84 51.84
	837	CB	LEU	105	42.199	33.440	42.086	1.00	27.36
5	838 839	CQ: CD1	LEU	105	41.385	34.348	42.989	1.00	27.36
,	840	CD2	LEU	105 105	40.132 40.988	34.710 33.638	42.214	1.00	27.36
	841	C	LEU	105	43.897	31.690	44.293 41.857	1.00 1.00	27.36
	842	0	LEU	105	44.802	31.948	41.068	1.00	51.84 51.84
10	843	N	ARG	106	43.337	30.499	41.929	1.00	60.02
10	844	CA CB	ARG	106	43.820	29.474	41.063	1.00	60.02
	845 846	CG	ARG ARG	106 106	44.949 45.476	28.740	41.722	1.00	28.53
	847	CD	ARG	106	46.314	27.618 26.830	40.886 41.814	1.00 1.00	28.53
	848	NE	ARG	106	47.260	25.934	41.174	1.00	28.53 28.53
15	849	CZ	ARG	106	47.904	25.010	41.864	1.00	28.53
	850	NH1	ARG	106	47.633	24.925	43.173	1.00	28.53
	851 852	NH2 C	ARG ARG	106 106	48.819	24.231	41.267	1.00	28.53
	853	ŏ	ARG	106	42.775 42.121	28.496 27.884	40.663	1.00	60.02
20	854	Ň	CYS	107	42.625	28.378	41.498 39.353	1.00 1.00	60.02 30.47
	855	CA	CYS	107	41.692	27.449	38.763	1.00	30.47
	856	Ç :	CYS	107	42.484	26.168	38.645	1.00	30.47
	857	0	CYS	107	43.098	25.892	37.607	1.00	30.47
25	858 859	CB SG	CYS CYS	107	41.261	27.937	37.398	1.00	52.55
23	860	N N	HIS	107 108	39.630 42.476	27.258	36.984	1.00	52.55
	861	CA	HIS	108	43.224	25.399 24.162	39. 733 39. 80 8	1.00 1.00	44.34
	862	CB	HIS	108	43.644	23.916	41.229	1.00	44.34 41.81
20	863	ÇG	HIS	108	44.610	22.800	41.351	1.00	41.81
30	864	CD2	HIS	108	44.648	21.734	42.178	1.00	41.81
	865 866	ND1 CE1	HIS	108	45.701	22.686	40.519	1.00	41.81
	867	NE2	HIS HIS	108 108	46.370 45.753	21.595 20. 99 9	40.832	1.00	41.81
	868	C	HIS	108	43.753 42.526	20.999 22.934	41.835 39.310	1.00 1.00	41.81
35	869	0	HIS	108	41.515	22.530	39. 83 8	1.00	44.34 44.34
	870	N	GLY	109	43.084	22.315	38.293	1.00	45.07
	871	CA	GLY	109	42.461	21.121	37.772	1.00	45.07
	872 873	C	GLY	109	42.909	19.890	38.534	1.00	45.07
40	874	Ň	TRP	109 110	44.015 42.026	19.831 18.902	39.097	1.00	45.07
	875	CA	TRP	110	42.293	17.641	38. 56 5 39.239	1.00 1.00	46.18 46.18
	876	СВ	TRP	110	41.156	16.653	38.932	1.00	36.88
	877	CG	TRP	110	41.347	15.329	39.576	1.00	36.88
45	878	CD2	TRP	110	41.040	15.001	40.923	1.00	36.88
43	879 880	CE2 CE3	TRP TRP	110	41.526	13.697	41.176	1.00	36.88
	881	CD1	TRP	110 110	40.388 41.989	15.690 14.231	41.973	1.00	36.88
	882	NE1	TRP	110	42.110	13.251	39.047 39.999	1.00 1.00	36.88
	883	CZ2	TRP ·	110	41.408	13.055	42.401	1.00	36.88 36.88
50	884	CZ3	TRP	110	40.264	15.061	43.204	1.00	36.88
	885	CH2	TRP	110	40.773	13.748	43.408	1.00	36.88
	886 887	CO	TRP	110	43.615	17.100	38.726	1.00	46.18
	888	Ň	TRP ARG	110 111	43.910 44.416	17.235	37.539	1.00	46.18
55	889	ČA	ARG	111	45.704	16.510 15.952	39. 60 9 39. 200	1.00 1.00	63.08
	890	CB	ARG	111	45.488	14.690	38.373	1.00	63.08 97.96
	891	CG	ARG	111	44.790	13.594	39.132	1.00	97.96
	892	CD	ARG	111	45.652	13.108	40.265	1.00	97.96
60	893 894	NE CZ	ARG	111	46.850	12.447	39.758	1.00	97.96
00	895	NH1	ARG ARG	111 111	47.845 47.785	12.019	40.528	1.00	97.96
	896	NH2	ARG	111	48.894	12.190 11.413	41.846 39.982	1.00 1.00	97.96
	897	C	ARG	111	46.465	16.961	38.358	1.00	97.96 63.08
<i>(</i>	898	0	ARG	111	47.152	16.596	37.406	1.00	63.08
65	899	N	ASN	112	46.324	18.237	38.685	1.00	111.35
	900 901	CA	ASN	112	47.011	19.247	37.914	1.00	111.35
	902	CB CG	ASN ASN	112 112	48.500	19.213	38.245	1.00	81.63
	903	OD1	ASN	112	48.814 48.719	19.880 21.101	39.568 39.701	1.00	81.63
70	904	ND2	ASN	112	49.182	19.082	39.701 40.556	1.00 1.00	81.63 81.63
				•			.0.500	1.00	01.03

	905 906	C	ASN ASN	112 112	46.791 47.744	18.987 18.946	36.424 35.648	1.00 1.00	111.35 111.35
	907	N.	TRP	113	45.540	18.783	36.027	1.00	91.49
5	908	CA	TRP	113	45.258	18.560	34.623	1.00	91.49
,	909 910	CB CG	TRP	113	43.894	17.929	34.393	1.00	88.74
	911	CD2	TRP TRP	113	43.813	16.506	34.706	1.00	88.74
	912	CE2	TRP	113 113	42.611	15.767	34.927	1.00	88.74
	913	CE3	TRP	113	42.998 41.258	14.439 16.105	35.200	1.00	88.74
10	914	CD1	TRP	113	44.845	15.625	34.927	1.00	88.74
	915	NE1	TRP	113	44.354	14.376	34.837 35.137	1.00	88.74
	916	CZ2	TRP	113	42.063	13.451	35.465	1.00 1.00	88.74
	917	CZ3	TRP	113	40.338	15.124	35.188	1.00	88.74
. ~	918	CH2	TRP	113	40.742	13.810	35.459	1.00	88.74 88.74
15	919	Ç	TRP	113	45.255	19.871	33.895	1.00	91.49
	920	0	TRP	113	44.941	20.922	34.463	1.00	91.49
	921	N	ASP	114	45.567	19.780	32.611	1.00	60.02
	922 923	CA CB	ASP ASP	114	45.599	20.940	31.755	1.00	60.02
20	924	CG	ASP	114	46.201	20.569	30.390	1.00	89.00
_0	925	OD1	ASP	114 114	47.637 48.360	20.066	30.498	1.00	89.00
	926	OD2	ASP	114	48.053	20.492 19.254	31.430	1.00	89.00
	927	C	ASP	114	44.210	21.555	29.643	1.00	89.00
	928	Ō	ASP	114	43.248	20.897	31.585 31.224	1.00	60.02
25	929	N	VAL	115	44.104	22.832	31.879	1.00 1.00	60.02
	930	CA	VAL	115	42.836	23.482	31.712	1.00	103.64 103.64
	931	CB	VAL	115	42.283	23.916	33.063	1.00	73.31
	932	CG1	VAL	115	40.951	24.620	32.902	1.00	73.31
30	933	CG2	VAL	115	42.153	22.682	33.943	1.00	73.31
30	934	C	VAL	. 115	43.127	24.647	30.805	1.00	103.64
	935 936	0 N	VAL	115	44.162	25.304	30.904	1.00	103.64
	937	CA	TYR TYR	116	42.232	24.861	29.868	1.00	59.95
	938	CB	TYR	116 116	42.415 42.503	25.932	28.943	1.00	59.95
35	939	ca	TYR	116	42.503 43.712	25.377 24.492	27.529	1.00	98.72
	940	CD1	TYR	116	43.675	23.152	27.362 27.726	1.00	98.72
	941	CE1	TYR	116	44.815	22.360	27.650	1.00 1.00	98.72
	942	CD2	TYR	116	44.922	25.017	26.914	1.00	98.72 98.72
40	943	CE2	TYR	116	46.067	24.233	26.839	1.00	98.72
40	944	CZ	TYR	116	46.008	22.908	27.207	1.00	98.72
	945	ОН	TYR	116	47.147	22.132	27.144	1.00	98.72
	946 947	. C	TYR	116	41.271	26.898	29.083	1.00	59.95
	948	N	TYR LYS	116	40.499	26.821	30.047	1.00	59.95
45	949	CA	LYS	117 117	41.176	27.814	28.127	1.00	66.79
	950	CB	LYS	117	40.132 38.946	28.813	28.132	1.00	66.79
	951	CG	LYS	117	37.902	28.332 29.406	27.295	1.00	151.68
	952	CD	LYS	117	38.475	30.515	27.008 26.129	1.00 1.00	151.68
~~	953	CE	LYS	117	37.451	31.604	25.848	1.00	151.68
50	954	NZ	LYS	117	38.062	32.685	25.034	1.00	151.68 151.68
	955	Ç	LYS	117	39.676	29.122	29.559	1.00	66.79
	956	0	LYS	117	38.472	29.233	29.810	1.00	66.79
	957 958	N	VAL	118	40.622	29.256	30.495	1.00	43.61
55	959	CA CB	VAL	118	40.243	29.564	31.879	1.00	43.61
55	960	CG1	VAL VAL	118	41.429	29.461	32.852	1.00	34.30
	961	CG2	VAL	118 118	40.912 42.246	29.485	34.289	1.00	34.30
	962	c	VAL	118	39.657	28.215 30.977	32.562	1.00	34.30
	963	Ō	VAL	118	40.002	31.881	31.998 31.235	1.00	43.61
60	964	N	ILE	119	38.772	31.168	32.963	1.00 1.00	43.61
	965	CA	ILE	119	38.135	32.458	33.140	1.00	47.57 47.57
	966	CB	ILE	119	36.895	32.621	32.203	1.00	48.87
	967	CG2	ILE	119	36.185	33.914	32.512	1.00	48.87
65	968	CG1	ILE	119	37.317	32.657	30.730	1.00	48.87
UJ.	969 970	CD1	ILE	119	36.187	33.009	29.752	1.00	48.87
	970	C	ILE	119	37.651	32.620	34.567	1.00	47.57
	972	N	ILE TYR	119	36.846	31.827	35.052	1.00	47.57
	973	CA	TYR	120 120	38.125	33.645	35.256	1.00	51.27
70	974	CB	TYR	120	37.647 38.727	33.835 34.342	36.608	1.00	51.27
					SO.1 E1	J-1.042	37.510	1.00	24.86

	975 976	CG CD1	TYR TYR	120 120	39.921 40.823	33.471 33.174	37.546 36.393	1.00	24.86
	977	CE1	TYR	120	41.794	32.429	36.448	1.00 1.00	24.86
_	978	CD2	TYR	120	40.397	33.004	38.754	1.00	24.86 24.86
5	979	CE2	TYR	120	41.562	32.258	38.832	1.00	24.86
	980	CZ	TYR	120	42.260	31.972	37.681	1.00	24.86
	981	ОН	TYR	120	43.423	31.233	37.816	1.00	24.86
	982 983	CO	TYR	120	36.531	34.832	36.621	1.00	51.27
10	984	N	TYR TYR	120 121	36.486	35.751	35.802	1.00	51.27
	985	CA	TYR	121	35.645 34.506	34.659 35.530	37.584 37.701	1.00	57.39
	986	CB	TYR	121	33.215	34.815	37.701 37.266	1.00 1.00	57.39
	987	CG	TYR	121	33.180	34.361	35.836	1.00	81.52 81.52
. ~	988	CD1	TYR	121	33.923	33.263	35.423	1.00	81.52
15	989	CE1	TYR	121	33.918	32.846	34.105	1.00	81.52
	990	CD2	TYR	121	32.419	35.042	34.889	1.00	81.52
	991 992	CE2 CZ	TYR	121	32.407	34.642	33.554	1.00	81.52
	993	OH	TYR TYR	121	33.163	33.537	33.171	1.00	81.52
20	994	C	TYR	121 121	33.195 34.315	33.117 35.966	31.859	1.00	81.52
	995	ŏ	TYR	121	34.522	35.184	39.124 40.054	1.00	57.39
	996	N	LYS	122	33.907	37.218	39.282	1.00 1.00	57.39
	997	CA	LYS	122	33.595	37.748	40.589	1.00	81.15 81.15
05	998	СВ	LYS	122	34.433	38.961	40.948	1.00	110.18
25	999	CG	LYS	122	34.253	39.334	42.403	1.00	110.18
	1000	CD	LYS	122	34.827	40.684	42.722	1.00	110.18
	1001 1002	CE NZ	LYS	122	33.834	41.772	42.392	1.00	110.18
	1002	C	LYS LYS	122 122	34.358	43.095	42.796	1.00	110.18
30	1004	ŏ	LYS	122	32.159 31.834	38.177 39.050	40.444	1.00	81.15
	1005	Ň	ASP	123	31.289	37.539	39. 64 2 41. 20 9	1.00 1.00	81.15
	1006	CA	ASP	123	29.875	37.861	41.159	1.00	100.05 100.05
	1007	CB	ASP	123	29.640	39.238	41.781	1.00	124.27
35	1008	CG	ASP	123	30.336	39.380	43.124	1.00	124.27
33	1009	OD1	ASP	123	30.145	38.499	43.991	1.00	124.27
	1010 1011	OD2	ASP	123	31.075	40.370	43.309	1.00	124.27
	1012	C	ASP ASP	123 123	29.401	37.816	39.720	1.00	100.05
	1013	Ň	GLY	123	29.086 29.407	38.844 36.612	39.125	1.00	100.05
40	1014	CA	GLY	124	28.929	36.423	39.157 37.803	1.00	103.70
	1015	C	GLY	124	29.750	37.084	36.729	1.00 1.00	103.70 103.70
	1016	0	GLY	124	29.983	36.517	35.684	1.00	103.70
	1017	N	GLU	125	30.231	38.285	37.011	1.00	86.80
45	1018	CA	GLU	125	31.033	39.025	36.046	1.00	86.80
43	1019 1020	CB	GLU	125	30.929	40.506	36.309	1.00	167.98
	1020	CD	GLU GLU	125 125	29.523	41.030	36.184	1.00	167.98
	1022	OE1	GLU	125	29.407 30.209	42.485 43.326	36.603	1.00	167.98
	1023	OE2	GLU	125	28.505	43.326 42.791	36.133 37.413	1.00	167.98
50	1024	c_	GLU	125	32.515	38.651	35.940	1.00 1.00	167.98
	1025	0	GLU	125	33.206	38.440	36.952	1.00	86.80 86.80
	1026	N	ALA	126	33.003	38.614	34.700	1.00	117.82
	1027	CA	ALA	126	34.395	38.279	34.411	1.00	117.82
55	1028 1029	СВ	ALA	126	34.627	38.310	32.891	1.00	16.51
<i>J</i> J	1030	CO	ALA	126	35.399	39.201	35.101	1.00	117.82
	1031	Ň	ALA LEU	126 127	35.141	40.384	35.284	1.00	117.82
	1032	ĊA	LEU	127	36.556 37.572	38.665 39.4 9 0	35.467 36.104	1.00	95.95
	1033	CB	LEU	127	38.604	38.639	36.840	1.00 1.00	95.95
60	1034	CG	LEU	127	38.205	37.916	38.119	1.00	46.01 46.01
	1035	CD1	LEU	127	39.484	37.355	38.754	1.00	46.01
	1036	CD2	LEU	127	37.491	38.848	39.082	1.00	46.01
	1037	C	LEU	127	38.281	40.327	35.050	1.00	95.95
65	1038 1039	0 N	LEU	127	38.475	39.885	33.911	1.00	95.95
00	1040	CA	LYS	128	38.664	41.538	35.450	1.00	158.42
	1041	CB	LYS LYS	128 128	39.342	42.486	34.573	1.00	158.42
	1042	ČĠ	LYS	128	39.220 37.787	43.899 44.386	35.142	1.00	155.76
=-	1043	CD	LYS	128	37.114	44.590	35.312 33.960	1.00 1.00	155.76 155.76
70	1044	CE	LYS	128	35.689	45.116	34.097	1.00	155.76
						-			155.70

	1045	NZ	LYS	128	35.067	45.392	32.766	1.00	155.76
	1046	Č	LYS	128	40.813	42.148	34.369	1.00	158.42
	1047	0	LYS	128	41.144	41.178	33.693	1.00	158.42
5	1048 1049	N	TYR	129	41.698	42.949	34.954	1.00	117.79
,	1050	CA CB	TYR TYR	129 129	43.132 43.851	42.714	34.800	1.00	117.79
	1051	cG	TYR	129	43.199	43.967 44.664	34.297 33.137	1.00	165.79
	1052	CD1	TYR	129	42.151	45.563	33.344	1.00 1.00	165.79
	1053	CE1	TYR	129	41.561	46.234	32.280	1.00	165.79 165.79
10	1054	CD2	TYR	129	43.643	44.447	31.832	1.00	165.79
	1055	CE2	TYR	129	43.060	45.112	30.759	1.00	165.79
	1056	CZ	TYR	129	42.022	46.005	30.991	1.00	165.79
	1057 1058	OH C	TYR	129	41.451	46.671	29.932	1.00	165.79
15	1059	ŏ	TYR TYR	129 129	43.834 44.261	42.279	36.077	1.00	117.79
10	1060	Ň	TRP	130	43.956	43.117 40.972	36.875 36.267	1.00 1.00	117.79
	1061	CA	TRP	130	44.647	40.433	37.422	1.00	50.95 50.95
	1062	CB	TRP	130	43.933	39.172	37.899	1.00	147.57
00	1063	CG	TRP	130	42.728	39.505	38.701	1.00	147.57
20	1064	CD2	TRP	130	42.410	39.002	39.993	1.00	147.57
	1065 1066	CE2	TRP	130	41.230	39.650	40.406	1.00	147.57
	1067	CE3 CD1	TRP TRP	130	43.023	38.088	40.853	1.00	147.57
	1068	NE1	TRP	130 130	41.744 40.841	40.394 40.486	38.378	1.00	147.57
25	1069	CZ2	TRP	130	40.636	39.388	39.400 41.632	1.00 1.00	147.57
	1070	CZ3	TRP	130	42.436	37.831	42.068	1.00	147.57 147.57
	1071	CH2	TRP	130	41.257	38.488	42.454	1.00	147.57
	1072	Ç	TRP	130	46.011	40.129	36.846	1.00	50.95
30	1073	0	TRP	130	46.184	40.232	35.628	1.00	50.95
30	1074	N	TYR	131	46.980	39.759	37.670	1.00	143.97
	1075 1076	CA CB	TYR TYR	131 131	48.287	39.493	37.101	1.00	143.97
	1077	CG	TYR	131	49.320 50.636	39.136 38.736	38.170 37.544	1.00	125.03
	1078	CD1	TYR	131	51.129	39.426	36.443	1.00 1.00	125.03 125.03
35	1079	CE1	TYR	131	52.276	39.026	35.794	1.00	125.03
	1080	CD2	TYR	131	51.347	37.634	37.995	1.00	125.03
	1081	CE2	TYR	131	52.511	37.230	37.352	1.00	125.03
	1082	CZ	TYR	131	52.964	37.927	36.249	1.00	125.03
40	1083 1084	OH C	TYR TYR	131	54.078	37.504	35.573	1.00	125.03
10	1085	ŏ	TYR	131 131	48.285 48.818	38.404 38.608	36.033 34.943	1.00	143.97
	1086	Ň	GLU	132	47.700	37.254	36.351	1.00 1.00	143.97 105.73
	1087	CA	GLU	132	47.628	36.119	35.427	1.00	105.73
	1088	СВ	GLU	132	47.113	36.560	34.053	1.00	172.31
45	1089	CG	GLU	132	46.992	35.425	33.034	1.00	172,31
	1090 1091	CD	GLU	132	46.449	35.896	31.695	1.00	172.31
	1092	OE1 OE2	GLU GLU	132	45.321	36.436	31.670	1.00	172.31
	1093	C	GLU	132 132	47.148 48.962	35.724 35.397	30.670	1.00	172.31
50	1094	ŏ	GLU	اند اند	50.022	35.935	35.256 35.552	1.00 1.00	105.73 105.73
	1095	N	ASN	133	48.887	34.172	34.758	1.00	117.87
	1096	CA	ASN	1 3 3	50.061	33.336	34.554	1.00	117.87
	1097	CB	ASN	133	50.894	33.311	35.844	1.00	184.60
55	1098	CG	ASN	133	52.234	32.621	35.675	1.00	184.60
33	1099 1100	OD1 ND2	ASN	133	52.612	32.227	34.573	1.00	184.60
	1101	C	ASN ASN	133 133	52.966 49.470	32.479	36.775	1.00	184.60
	1102	ŏ	ASN	133	48.297	31.961 31.741	34.285 34.563	1.00 1.00	117.87 117.87
	1103	Ň	HIS	134	50.248	31.038	33.732	1.00	156.61
60	1104	CA	HIS	134	49.714	29.700	33.509	1.00	156.61
	1105	CB	HIS	134	50.697	28.835	32.710	1.00	161.49
	1106	CG	HIS	134	50.137	27.491	32.325	1.00	161.49
	1107 1108	CD2	HIS	134	50.423	26.249	32.787	1.00	161.49
65	1109	ND1 CE1	.HIS HIS	134 134	49.130	27.348 26.061	31.409	1.00	161.49
	1110	NE2	HIS	134	48.802 49.569	25.382	31.313 32.136	1.00	161.49
	1111	C	HIS	134	49.547	29.124	34.915	1.00 1.00	161.49 156.61
	1112	0	HIS	134	49.172	27.967	35.093	1.00	156.61
70	1113	N	ASN	135	49.821	29.965	35.910	1.00	97.51
70	1114	CA	ASN	135	49.755	29.570	37.304	1.00	97.51

	1115	CB	ASN	135	51.160	29.704	37.934	1.00	110.39
	1116	CG	ASN	135	52.230	28.875	37.217	1.00	110.39
	1117 1118	OD1 ND2	ASN ASN	135 135	51.990 53.438	27.742	36.801	1.00	110.39
5	1119	C	ASN	135	48.729	29.433 30.282	37.117 38.193	1.00	110.39
_	1120	ŏ	ASN	135	48.097	29.646	39.031	1.00 1.00	97.51
	1121	N	ILE	136	48.542	31.589	38.037	1.00	97.51 101.73
	1122	CA	ILE	136	47.600	32.267	38.943	1.00	101.73
10	1123	СВ	ILE	136	48.307	32.728	40.212	1.00	31.25
10	1124	CG2	ILE	136	47.296	33.031	41.311	1.00	31.25
	1125 1126	CG1 CD1	ILE	136	49.240	31.649	40.728	1.00	31.25
	1127	C	ILE	136	49.753	31.893	42.146	1.00	31.25
	1128	ŏ	ILE	136 136	46.867 46.274	33.476 33.477	38.424	1.00	101.73
15	1129	Ň	SER	137	46.901	34.498	37.354 39.257	1.00 1.00	101.73
	1130	CA	SER	137	46.286	35.780	39.011	1.00	57.41 57.41
	1131	СВ	SER	137	44.901	35.617	38.380	1.00	67.48
	1132	<u>o</u> G	SER	137	44.052	35.011	39.328	1.00	67.48
20	1133	C	SER	137	46.183	36.488	40.392	1.00	57.41
20	1134 1135	0 N	SER	137	45.619	35.936	41.348	1.00	57.41
	1136	ČA	ILE	138 138	46.730	37.708	40.476	1.00	65.35
	1137	CB	ILE	138	46.751 48.186	38.515 38.693	41.708	1.00	65.35
	1138	CG2	ILE	138	48.232	39.050	42.184 43.659	1.00 1.00	90.30
25	1139	CG1	ILE	138	48.941	37.407	41.930	1.00	90.30 90.30
	1140	CD1	ILE	138	50.416	37.583	41.970	1.00	90.30
	1141	C	ILE	138	46.148	39.928	41.561	1.00	65.35
	1142	0	ILE	138	46.060	40.471	40.456	1.00	65.35
30	1143 1144	N	THR	139	45.745	40.515	42.683	1.00	86.56
50	1145	CA CB	THR THR	139	45.164	41.843	42.672	1.00	86.56
	1146	OG1	THR	139 139	43.649 43.399	41.817 41.192	42.377	1.00	127.73
	1147	CG2	THR	139	43.093	43.253	41.115 42.386	1.00 1.00	127.73
	1148	C	THR	139	45.331	42.466	44.043	1.00	127.73 86.56
35	1149	0	THR	139	45.198	41.779	45.051	1.00	86.56
	1150	N	ASN	140	45.624	43.763	44.089	1.00	96.52
	1151	CA	ASN	140	45.753	44.415	45.370	1.00	96.52
	1152 1153	CB CG	ASN ASN	140	46.301	45.834	45.214	1.00	124.36
40	1154	OD1	ASN	140 140	46.721 46.321	46.427 45.925	46.534	1.00	124.36
	1155	ND2	ASN	140	47.512	45.825 47.492	47.576 46.515	1.00	124.36
	1156	C	ASN	140	44.325	44.432	45.916	1.00 1.00	124.36 96.52
	1157	0	ASN	140	43.390	44.861	45.244	1.00	96.52
45	1158	N	ALA	141	44.168	43.921	47.126	1.00	84.53
45	1159	CA	ALA	141	42.876	43.846	47.769	1.00	84.53
	1160 1161	CB C	ALA	141	43.022	43.170	49.104	1.00	49.12
	1162	ŏ	ALA ALA	141 141	42.197 42.778	45.188	47.942	1.00	84.53
	1163	Ň	THR	142	40.942	46.143 45.223	48.459	1.00	84.53
50	1164	CA	THR	142	40.094	46.401	47.514 47.593	1.00 1.00	86.11 86.11
	1165	CB	THR	142	39.660	48.860	46.184	1.00	85.26
	1166	OG1	THR	142	40.816	47.143	45.386	1.00	85.26
	1167	CG2	THR	142	38.793	48.102	46.268	1.00	85.26
55	1168	C	THR	142	38.847	45.9 5 5	48.337	1.00	86.11
33	1169 1170	0 N	THR	142	38.577	44.766	48.411	1.00	86.11
	1171	CA	VAL VAL	143 143	38.089 36.8 63	46.889 46.404	48.897	1.00	, u5.48
	1172	CB	VAL	143	36.240	46.494 47.653	49.566 50.360	1.00	105.48
	1173	CG1	VAL	143	35.816	48.766	49.413	1.00 1.00	154.19 154.19
60	1174	CG2	VAL	143	35.055	47.144	51.159	1.00	154.19
	1175	Ç	VAL	143	35.917	46.092	48.428	1.00	105.48
	1176	0	VAL	143	34.937	45.371	48.635	1.00	105.48
	1177	N CA	GLU	144	36.238	46.560	47.223	1.00	97.40
65	1178 1179	CA CB	GLU	144	35.454	46.269	46.022	1.00	97.40
55	1180	CG	GLU	144 144	35.815 35.304	47.241 48.845	44.905	1.00	151.67
	1181	CD	GLU	144	35.772	48.645 49.574	45.100	1.00	151.67
	1182	OE1	GLU	144	35.580	49.236	44.000 42.811	1.00 1.00	151.67 151.67
70	1183	OE2	GLU	144	36.330	50.643	44.324	1.00	151.67
70	1184	С	GLU	144	35.682	44.857	45.517	1.00	97.40

	1185 1186	0 N	GLU ASP	144	34.784	44.232	44.963	1.00	97.40
	1187	CA	ASP	145 145	36.905 37.266	44.376 43.040	45.690 45.268	1.00	99.27
	1188	CB	ASP	145	38.759	42.808	45.268 45.491	1.00 1.00	99.27
5	1189	CG	ASP	145	39.616	43.652	44.576	1.00	103.93 103.93
	1190	OD1	ASP	145	39.333	43.649	43.359	1.00	103.93
	1191	OD2	ASP	145	40.568	44.306	45.064	1.00	103.93
	1192	C	ASP	145	36.461	42.016	46.042	1.00	99.27
10	1193 1194	. O	ASP SER	145 146	36.442	40.847	45.687	1.00	99.27
10	1195	CA	SER	146	35.793 34.985	42.455 41.545	47.104 47.900	1.00 1.00	71.52
	1196	СВ	SER	146	34.386	42,266	49.105	1.00	71.52 85.74
	1197	OG	SER	146	35.371	42.424	50.111	1.00	85.74
15	1198	C	SER	146	33.900	40.948	47.012	1.00	71.52
15	1199 1200	0	SER	146	33.469	41.569	46.036	1.00	71.52
	1200	N CA	GLY GLY	147 147	33.493	39.724	47.333	1.00	96.87
	1202	Č.	GLY	147	32.481 32.739	39.051 37.567	46.546 46.394	1.00	96.87
	1203	ŏ	GLY	147	33.695	CT 032	46.955	1.00 1.00	96.87 96.87
20	1204	N	THR	148	31.883	26.908	45.617	1.00	103.30
	1205	CA	THR	148	31.975	35.469	45.377	1.00	103.30
	1206 1207	CB OG1	THR	148	30.596	34.819	45.355	1.00	64.66
	1208	CG2	THR THR	148 148	30.231	34.568	43.990	1.00	64.66
25	1209	C	THR	148	29.559 32.629	35.746 35.167	45.982 44.035	1.00 1.00	64.66
	1210	Ō	THR	148	32.261	35.726	42.998	1.00	103.30 103.30
	1211	N	TYR	149	33.586	34.253	44.059	1.00	77.50
	1212	CA	TYR	149	34.294	33.888	42.853	1.00	77.50
30	1213	CB	TYR	149	35.798	34.053	43.059	1.00	78.57
50	1214 1215	CG CD1	TYR TYR	149 149	36.237 35.965	35.491	43.209	1.00	78.57
	1216	CE1	TYR	149	36.349	36.210 37.540	44.372 44.492	1.00 1.00	78.57
	1217	CD2	TYR	149	36.907	36.141	42.169	1.00	78.57 78.57
~~	1218	CE2	TYR	149	37.291	37.463	42.277	1.00	78.57.
35	1219	CZ	TYR	149	37.012	38.161	43.437	1.00	78.57
	1220 1221	ОН	TYR	149	37.388	39.485	43.527	1.00	78.57
	1222	C	TYR TYR	149 149	34.018 33.424	32.469 31.694	42.439	1.00	77.50
	1223	Ň	TYR	150	34.473	32.150	43.185 41.232	1.00 1.00	77.50 44.44
40	1224	CA	TYR	150	34.335	30.823	40.648	1.00	44.44
	1225	CB	TYR	150	32.851	30.446	40.588	1.00	66.36
	1226	CG	TYR	150	32.132	30.968	39.376	1.00	66.36
	1227 1228	CD1 CE1	TYR TYR	150 150	32.205	30.288	38.157	1.00	66.36
45	1229	CD2	TYR	150	31.585 31.411	30.776 32.156	37.034 39.433	1.00 1.00	66.36
	1230	CE2	TYR	150	30.788	32.655	38.315	1.00	66.36 66.36
	1231	CZ	TYR	150	30.878	31.959	37.120	1.00	66.36
	1232	ÓН	TYR	150	30.243	32.436	36.007	1.00	66.36
50	1233 1234	C	TYR TYR	150	34.957	30.881	39.240	1.00	44.44
50	1235	Ň	CYS	150 151	34.796 35.677	31.872 29.842	38.536	1.00	44.44
	1236	ĊA	CYS	151	36.290	29.853	38.833 37.513	1.00 1.00	64.10 64.10
	1237	С	CYS	151	35.713	28.792	36.616	1.00	64.10
55	1238	0_	CYS	151	35.015	27.897	37.067	1.00	64.10
55	1239	CB	CYS	151	37.813	29.668	37.612	1.00	75.24
	1240 1241	SG N	THR	151	38.407	28.123	38.380	1.00	75.24
	1242	ĞA	THR	152 152	36.021 35.553	28.904 27.971	35.334 34.330	1.00	63.66
	1243	CB	THR	152	34.453	28.599	33.459	1.00 1.00	63.66 48.15
60	1244	OG1	THR	152	35.025	29.615	32.619	1.00	48.15
	1245	CG2	THR	152	33.360	29.204	34.341	1.00	48.15
	1248 1247	C	THR	152	36.779	27.708	33.479	1.00	63.66
	1247	0 N	THR GLY	152 153	37.709 38.786	28.512	33.473	1.00	63.66
65	1249	ČA	GLY	153	36.786 37.917	26.586 26.256	32.770 31.929	1.00 1.00	68.75
	1250	Č	GLY	153	37.588	24.988	31.180	1.00	68.75 68.75
	1251	0	GLY	153	36.783	24.186	31.649	1.00	68.75
	1252	N	LYS	154	38.192	24.800	30.016	1.00	56.66
70	1253 1254	CA CB	LYS	154	37.936	23.603	29.248	1.00	56.66
, 5	1207	Ç.	LYS	154	37.984	23.917	27.751	1.00	131.33

	1255	CG	LYS	154	37.756	22.699	00.074	4.00	
	1256	CD	LYS	154	38.014	22.985	26.874 25.401	1.00 1.00	131.33
	1257	CE ·	LYS	154	37.989	21.684	24.596	1.00	131.33
	1258	NZ	LYS	154	38.322	21.823	23.146	1.00	131.33 131.33
5	1259	C	LYS	154	38.932	22.501	29.582	1.00	56.66
	1260	0	LYS	154	40.141	22.713	29.562	1.00	56.66
	1261	N	VAL	155	38.412	21.321	29.913	1.00	93.07
	1262	CA	VAL	155	39.260	20.162	30.203	1.00	93.07
10	1263	CB	VAL	155	38.924	19.490	31.544	1.00	78.48
10	1264	CG1	VAL	155	40.072	18.590	31.955	1.00	78.48
	1265	CG2	VAL	155	38.659	20.536	32.606	1.00	78.48
	1266	C	VAL	155	38.956	19.179	29.095	1.00	93.07
	1267 1268	Ň	VAL TRP	155 156	37.802 39.992	19.005 18.547	28.719	1.00	93.07
15	1269	ČA	TRP	156	39.826	17,597	28.566 27.476	1.00	110.90
10	1270	CB	TRP	156	39.093	16.344	27.476 27.963	1.00 1.00	110.90
	1271	CG	TRP	156	39.889	15.530	28.952	1.00	64.42 64.42
	1272	CD2	TRP	156	41.144	14.909	28.711	1.00	64.42
	1273	CE2	TRP	156	41.538	14.254	29.912	1.00	64.42
20	1274	CE3	TRP	156	41.989	14.836	27.593	1.00	64.42
	1275	CD1	TRP	156	39.562	15.241	30.265	1.00	64.42
	1276	NE1	TRP	156	40.550	14.478	30.845	1.00	64.42
	1277	CZ2	TRP	156	42.732	13.535	30.029	1.00	64.42
25	1278	CZ3	TRP	156	43.178	14.125	27.705	1.00	64.42
25	1279 1280	CH2	TRP	156	43.539	13.482	28.919	1.00	64.42
	1281	C	TRP	156 156	39.063 39.674	18.269	26.335	1.00	110.90
	1282	Ň	GLN	157	37. 73 8	18.848 18.225	25.432	1.00	110.90
	1283	CA	GLN	157	36.980	18.857	26.366 25. 2 98	1.00 1.00	82.18 82.18
30	1284	CB	GLN	157	36.566	17.802	24.260	1.00	143.76
	1285	CG	GLN	157	37.656	16.778	23.860	1.00	143.76
	1286	CD	GLN	157	37.147	15.761	22.835	1.00	143.76
	1287	OE1	GLN	157	35.954	15.470	22.790	1.00	143.76
25	1288	NE2	GLN	157	38.050	15.211	22.025	1.00	143.76
35	1289	Ç	GLN	157	35.737	19.520	25.889	1.00	82,18
	1290 1291	0	GLN	157	34.910	20.068	25.166	1.00	82.18
	1292	N CA	LEU	158	35.620	19.488	27.213	1.00	73.39
	1293	CB	LEU	158 158	34.443 33.835	20.030 18.977	27.881	1.00	73.39
40	1294	CG	LEU	158	34.030	17.598	28. 77 3 28.187	1.00 1.00	92.19
	1295	CD1	LEU	158	33.153	16.628	28.944	1.00	92.19 92.19
	1296	CD2	LEU	158	33.664	17.618	26.702	1.00	92.19
	1297	C	LEU	158	34.658	21.254	28.724	1.00	73.39
	1298	0	LEU	158	35.763	21.525	29.180	1.00	73.39
45	1299	N	ASP	159	33.564	21.955	28.992	1.00	13.69
	1300	CA	ASP	159	33.615	23.183	29.761	1.00	43.69
	1301	CB	ASP	159	32.773	24.249	29.074	1.00	96.10
	1302 1303	CG OD1	ASP ASP	159	33.085	24.373	27.594	1.00	86.10
50	1304	OD2	ASP	159 159	34.289 32.128	24.477 24.374	27.249	1.00	86.10
-	1305	C	ASP	159	33.103	23.041	26.778 31.167	1.00	86.10
	1306	ŏ	ASP	159	31.900	22.907	31.167	1.00 1.00	43.69 43.69
	1307	N	TYR	160	33.976	23.093	32.170	1.00	43.37
	1308	CA	TYR	160	33.462	22.999	33.539	1.00	43.37
55	1309	CB	TYR	160	34.282	22.024	34.398	1.00	105.78
	1310	CG	TYR	160	34.323	20.649	33.808	1.00	105.78
	1311	CD1	TYR	160	35.087	20.415	32.671	1.00	105.78
	1312	CE1	TYR	160	35.035	19.211	32.001	1.00	105.78
60	1313 1314	CD2 CE2	TYR	160	33.500	19.617	34.286	1.00	105.78
00	1315	CZ	TYR TYR	160	33.436	18.387	33.612	1.00	105.78
	1316	OH	TYR	160 160	34.209 34.143	18.205	32.458	1.00	105.78
	1317	C	TYR	160	33.340	17.068 24.331	31.692 34.265	1.00	105.78
	1318	ŏ	TYR	160	33.620	25.407	34.265 33.736	1.00 1.00	43.37 43.37
65	1319	Ň	GLU	161	32.893	24.230	35.498	1.00	53.88
	1320	CA	GLU	161	32.709	25.388	36.333	1.00	53.88
	1321	СВ	GLU	161	31.270	25.866	36.228	1.00	72.58
	1322	ca	GLU	161	30.834	26.756	37.346	1.00	72.58
70	1323	CD	GLU	161	29.490	27.372	37.067	1.00	72.58
70	1324	OE1	GLU	161	28.930	28.016	37.992	1.00	72.58

	1325	OE2	GLU	161	29.002	27.212	35.918	1.00	70.50
	1326	C	GLU	161	33.002	24.902	37.725	1.00	72.58 53.88
	1327	0	GLU	161	32.658	23.765	38.063	1.00	53.88
5	1328 1329	N	SER	162	33.651	25.737	38.523	1.00	54.33
,	1330	CA CB	SER SER	162 162	33.967 35.289	25.330 25.931	39.868	1.00	54.33
	1331	OG	SER	162	35.183	27.339	40.327 40.452	1.00 1.00	58.04
	1332	Ċ	SER	162	32.868	25.781	40.794	1.00	58.04 54.33
10	1333	0	SER	162	31.975	26.508	40.391	1.00	54.33
10	1334	N	GLU	163	32.923	25.298	42.028	1.00	45.72
	1335 1336	CA CB	GLU GLU	163 163	31.959	25.656	43.045	1.00	45.72
	1337	CG	GLU	163	32.210 31.766	24.853 23.437	44.313 44.264	1.00	129.00
	1338	CD	GLU	163	30.264	23.378	44.300	1.00 1.00	129.00 129.00
15	1339	OE1	GLU	163	29.702	24.206	45.051	1.00	129.00
	1340	OE2	GLU	163	29.657	22.531	43.595	1.00	129.00
	1341 1342	C	GLU	163	32.259	27.102	43.356	1.00	45.72
	1343	N	GLU PRO	163 164	33.425 31.219	27.501 27.914	43.399	1.00	45.72
20	1344	CD	PRO	164	29.759	27.742	43.576 43.567	1.00 1.00	67.32
	1345	CA	PRO	164	31.578	29.289	43.884	1.00	86.92 67.32
	1346	CB	PRO	164	30.227	29.992	43.934	1.00	86.92
	1347	cg	PRO	164	29.312	28.921	44.383	1.00	86.92
25	1348 1349	C	PRO	164	32.342	29.348	45.213	1.00	67.32
23	1350	N	PRO LEU	164 165	32.402 32.943	28.372	45.973	1.00	67.32
	1351	CA	LEU	165	33.699	30.507 30.751	45.461 46.675	1.00 1.00	65.83
	1352	CB	LEU	165	35.183	30.549	46.392	1.00	65.83 49.81
20	1353	CG	LEU	165	36.123	30.662	47.579	1.00	49.81
30	1354	CD1	LEU	165	35.645	29.788	48.747	1.00	49.81
	1355 1356	CD2	LEU	165	37.495	30.247	47.100	1.00	49.81
	1357	C	LEU	165 165	33.424	32.177	47.156	1.00	65.83
	1358	Ň	ASN	166	33.235 33.376	33.094 32.358	46.344 48.473	1.00	65.83
35	1359	CA	ASN	166	33.117	33.676	49.033	1.00 1.00	106.87 106.87
	1360	CB	ASN	166	31.975	33.597	50.055	1.00	138.19
	1361	CG	ASN	166	30.601	33.541	49.380	1.00	138.19
	1362 1363	OD1 ND2	ASN	166	30.053	32.448	49.150	1.00	138.19
40	1364	C	ASN ASN	166 166	30.075 34.356	34.724 34.348	49.034	1.00	138.19
	1365	ŏ	ASN	166	34.960	33.853	49.629 50.578	1.00 1.00	106.87
	1366	N	ILE	167	34.719	35.487	49.041	1.00	106.87 79.40
	1367	CA	ILE	167	35.882	36.278	49.444	1.00	79.40
45	1368	CB	(LE	167	36.849	36.419	48.260	1.00	72.10
43	1369 1370	CG2 CG1	担用	167	37.796	37.571	48.491	1.00	72.10
	1371	CD1	ILE	167 167	37.558 38.444	35.074 35.007	48.042	1.00	72.10
	1372	Č.	ILE	167	35.502	37.662	46.826 49.951	1.00 1.00	72.10 79.40
50	1373	0	ILE	167	34.768	38.397	49.295	1.00	79.40 79.40
50	1374	N	THR	168	36.013	38.003	51.126	1.00	78.85
	1375 1376	CA	THR	168	35.727	39.284	51.750	1.00	78.85
	1377	CB OG1	THR	168	34.988	39.074	53.096	1.00	110.41
	1378	CG2	THR	168 168	33.724 34.753	38. 444 40.400	52.850 53.805	1.00	110.41
55	1379	C	THR	168	37.012	40.064	52.000	1.00 1.00	110.41 78.85
	1380	0	THR	168	37.999	39.523	52.508	1.00	78.85
	1381	N	VAL	169	36.997	41.338	51.634	1.00	91.78
	1382 1383	CA CB	VAL	169	38.163	42.177	51.829	1.00	91.78
60	1384	CG1	VAL. VAL	169 169	38.475 39.886	42.968 43.534	50.576	1.00	74.43
	1385	CG2	VAL	169	38.303	43.524 42.079	50.663 49.361	1.00	74.43
	1386	C	VAL	169	37.898	43.146	52.965	1.00 1.00	74.43 91.78
	1387	0	VAL	169	37.524	44.297	52.738	1.00	91.78
65	1388	N	ILE	170	38.085	42.676	54.192	1.00	138.54
UJ	1389 1390	CA CB	ILE	170	37.838	43.522	55.342	1.00	138.54
	1390	CB CG2	ILE ILE	170	38.201	42.815	56.649	1.00	99.90
	1392	CG1	ILE	170 170	38.104 37.253	43.798 41.628	57.810	1.00	99.90
	.1393	CD1	ILE	170	37.436	40.914	56.869 58.193	1.00 1.00	99.90
70	1394	C	ILE	170	38.598	44.837	55.255	1.00	99.90 138.54

	1395 1396	O N	ILE LYS	170 171	39.816 37.856	44.880 45.912	55.419 55.002	1.00	138.54
	1397	CA ·	LYS	171	38.420	47.254	54.878	1.00	166.26
	1398	CB .	LYS	171	37.322	48.228	54. 43 0	1.00 1.00	166.26
5	1399	CG	LYS	171	37.806	49.608	53.987	1.00	153.43 153.43
	1400	CD	LYS	171	36.637	50.449	53.489	1.00	153.43
	1401	CE	LYS	171	37.084	51.765	52.885	1.00	153.43
	1402	NZ	LYS	171	35.907	52.541	52.405	1.00	153.43
• •	1403	С	LYS	171	39.042	47.737	56.189	1.00	166.26
10	1404	0	LYS	171	39.710	46.977	56.894	1.00	166.26
	1405	C1	NAG	221	52.176	13.407	48.424	1.00	124.69
	1406	C2	NAG	221	52.353	13.121	46.936	1.00	124.69
	1407 1408	N2 C7	NAG	221	51.119	13.440	46.226	1.00	124.69
15	1409	07	NAG NAG	221 221	51.096 52.111	14.392	45.292	1.00	124.69
13	1410	C8	NAG	221	49.744	14.981 14.746	44.911	1.00	124.69
	1411	C3	NAG	221	52.712	11.631	44. 6 82 46. 75 3	1.00 1.00	124.69
	1412	03	NAG	221	53.109	11.400	45.409	1.00	124.69
	1413	C4	NAG	221	53.847	11.168	47.703	1.00	124.69 124.69
20	1414	04	NAG	221	53.876	9.724	47.741	1.00	124.69
	1415	C5	NAG	221	53.635	11.683	49.139	1.00	124.69
	1416	05	NAG	221	53.371	13.099	49.133	1.00	124.69
	1417	C6	NAG	221	54.853	11.458	50.023	1.00	124.69
25	1418	06	NAG	221	54.616	11.876	51.361	1.00	124.69
23	1419 1420	C1 C2	NAG	222	55.008	9.074	47.260	1.00	186.41
	1421	N2	NAG NAG	222 222	55.394	7.926	48.219	1.00	186.41
	1422	C7	NAG	222	55.812 55.243	8.470 8.053	49.500	1.00	186.41
	1423	07	NAG	222	54.288	7.270	50.628 50.654	1.00	186.41
30	1424	C8	NAG	222	55.823	8.589	51. 93 0	1.00 1.00	186.41
	1425	СЗ	NAG	222	56.531	7.079	47.623	1.00	186.41 186.41
	1426	03	NAG	222	56.764	5.942	48.445	1.00	186.41
	1427	C4	NAG	222	56.174	6.622	46.205	1.00	186.41
25	1428	04	NAG	222	57.286	5.958	45.616	1.00	186.41
35	1429	C5	NAG	222	55.775	7.830	45. 34 5	1.00	186.41
	1430 1431	O5 C6	NAG	222	54.681	8.548	45.963	1.00	186.41
	1431	06	NAG NAG	222 222	55.302	7.412	43.963	1.00	186.41
	1433	C1	NAG	242	54.550 36.605	8.444 17.603	43.340	1.00	186.41
40	1434	C2	NAG	242	36.383	16.211	61.014 60.400	1.00	57.79
	1435	N2	NAG	242	37.564	15.387	60.550	1.00 1.00	57.79 57.79
	1436	C7	NAG	242	37.706	14.678	61.665	1.00	57.79
	1437	07	NAG	242	36.949	14.833	62.624	1.00	57.79
4.5	1438	C8	NAG	242	38.838	13.642	61.747	1.00	57.79
45	1439	C3	NAG	242	36.035	16.395	58.924	1.00	57.79
	1440	03	NAG	242	35.897	15.142	5 8.25 6	1.00	57.79
	1441 1442	C4 O4	NAG	242	34.754	17.226	58.828	1.00	57.79
	1443	C5	NAG NAG	242 242	34.498 34.988	17.491	57.446	1.00	57.79
50	1444	O5	NAG	242	35.393	18.570 18.365	59.547	1.00	57.79
•	1445	C6	NAG	242	33.781	19.492	60.921 59. 55 6	1.00 1.00	57.79
	1446	06	NAG	242	34.170	20.863	59.403	1.00	57.79 57.79
	1447	C1	NAG	243	33,499	16.811	56.792	1.00	110.47
	1448	C2	NAG	243	33.279	17.515	55.463	1.00	110.47
55	1449	N2	NAG	243	32.859	18.887	55.667	1.00	110.47
	1450	C7	NAG	243	33.584	19.876	55.149	1.00	110.47
	1451	07	NAG	243	34.659	19.682	54.574	1.00	110.47
	1452 1453	C8	NAG	243	33.036	21.294	55.277	1.00	110.47
60	1454	C3 O3	NAG NAG	243 243	32.273	16.758	54.610	1.00	110.47
OO	1455	64 64	NAG	243 243	32.168 32.746	17.391	53.345	1.00	110.47
	1456	04	NAG	243	31.718	15.314 14.574	54.413 52.705	1.00	110.47
	1457	C5	NAG	243	33.038	14.665	53.705 55.789	1.00 1.00	110.47 110.47
	1458	['] O5	NAG	243	33.967	15.474	56.555	1.00	110.47
65	1459	C6	NAG	243	33.671	13.290	55.655	1.00	110.47
	1460	Q6	NAG	243	34.005	12.749	56.924	1.00	110.47
	1461	C1	MAN	244	32.107	13.609	52.777	1.00	99.82
	1462	C2	MAN	244	31.311	12.313	53.039	1.00	99.82
70	1463 1464	02 C3	MAN	244	29.925	12.615	53.134	1.00	99.82
, 0	1-10-1	W	MAN	244	31.545	11.278	51.921	1.00	99.82

	1465 1466 1467	03 C4 04	MAN MAN MAN	244 244	30.713 31.266	10.135 11.903	52.110 50.555	1.00 1.00	99.82 99.82
	1468	C5 .	MAN	244 244	31.547 32.168	10.959	49.527	1.00	99.82
5	1469	OS	MAN	244	31.840	13.132 14.107	50.412	1.00	99.82
_	1470	C6	MAN	244	32,132	13.816	51.442 49.038	1.00	99.82
	1471	O6	MAN	244	30.954	14.583	48.837	1.00 1.00	99.82
	1472	C1	NAG	250	57.134	13.804	64.271	1.00	99.82
• •	1473	C2	NAG	250	57.130	13.286	65.723	1.00	196.94 196.94
10	1474	N2	NAG	250	58.492	13.078	66.175	1.00	196.94
	1475	C7	NAG	250	58.871	13.481	67.385	1.00	196.94
	1476 1477	O7 C8	NAG NAG	250	58.184	14.217	68.096	1.00	196.94
	1478	cs	NAG	250 250	60.225 56.359	12.994 11.960	67.883	1.00	196.94
15	1479	03	NAG	250	56.224	11.547	65.803 67.156	1.00	196.94
	1480	C4	NAG	250	54.974	12.098	65.176	1.00 1.00	196.94
	1481	04	NAG	250	54.343	10.826	65.136	1.00	196.94 196.94
	1482	C5	NAG	250	55.102	12.658	63.758	1.00	196.94
20	1483	O5	NAG	250	55.794	13.927	63.783	1.00	196.94
20	1484 1485	C6	NAG	250	53.754	12.893	63.115	1.00	196.94
	1486	O6 C1	NAG NAG	250 274	53.895	13.367	61.783	1.00	196.94
	1487	C2	NAG	274	45.966 44.449	34.168 34.481	75.904	1.00	202.51
	1488	N2	NAG	274	44.020	34.633	75.778 74.386	1.00	202.51
25	1489	C7	NAG	274	42.782	34.284	74.009	1.00 1.00	202.51
	1490	O7	NAG	274	42.000	33.685	74.755	1.00	202.51 202.51
	1491	C8	NAG	274	42.322	34.648	72.599	1.00	202.51
	1492	C3	NAG	274	44.167	35.773	76.602	1.00	202.51
30	1493 1494	O3 C4	NAG	274	42.768	35.996	76.692	1.00	202.51
50	1495	04	NAG NAG	274 274	44.757	35.723	78.040	1.00	202.51
	1496	C5	NAG	274	44.775 46.191	37.037 35.157	78.589	1.00	202,51
	1497	O5	NAG	274	46.265	33.950	78.058 77.282	1.00 1.00	202.51
٥.5	1498	C6	NAG	274	46.690	34.798	79.448	1.00	202.51 202.51
35	1499	O6	NAG	274	47.729	33.828	79.381	1.00	202.51
	1500	C1	NAG	340	47.734	48.240	47.742	1.00	87.46
	1501 1502	C2 N2	NAG	340	49.212	48.677	47.819	1.00	87.46
	1503	C7	NAG NAG	340 340	50.123 50. 634	47.546	47.707	1.00	87.46
40	1504	O7	NAG	340	50.025	47.210 47.375	46.522 45.468	1.00	87.46
	1505	C8	NAG	340	52.024	46.596	46.490	1.00 1.00	87.46 87.46
	1506	СЗ	NAG	340	49.416	49.457	49.129	1.00	87.46
	1507	03	NAG	340	50.779	49.830	49.261	1.00	87.46
45	1508 1509	C4	NAG	340	48.512	50.694	49.007	1.00	87.46
40	1510	O4 C5	NAG NAG	340 340	48.730	51.749	49.989	1.00	87.46
	1511	O5	NAG	340	47.044 46.834	50.277 49.391	48.965	1.00	87.46
	1512	C6	NAG	340	46.182	51.556	47.812 48. 7 93	1.00 1.00	87.46
	1513	O6	NAG	340	44.848	51.307	48.368	1.00	87.46 87.46
50	1514	C1	NAG	341	49.306	51.566	51.238	1.00	143.93
	1515	C2	NAG	341	50.167	52.801	51.506	1.00	143.93
	1516	N2	NAG	341	51.241	52.873	50.540	1.00	143.93
	1517 1518	C7 O7	NAG NAG	341	51.195	53.774	49.564	1.00	143.93
55	1519	C8	NAG	341 341	50.313 52.303	54.630 53.716	49.471	1.00	143,93
	1520	C3	NAG	341	50.722	53.716 52.777	48.535 52.923	1.00	143.93
	1521	Q 3	NAG	341	51.522	53.931	53.148	1.00 1.00	143.93 143.93
	1522	C4	NAG	341	49.548	52.753	53,891	1.00	143.93
60	1523	04	NAG	341	50.031	52.717	55.229	1.00	143.93
OU	1524	C5	NAG	341	48.686	51.510	53.587	1.00	143.93
	1525 1526	O5 C6	NAG	341	48.239	51.510	52.203	1.00	143.93
	1527	O6	NAG NAG	341 341	47.428 48.455	51.437	54.427	1.00	143.93
	1528	C1	NAG	366	46.455 28.633	50.627 34.916	53.780	1.00	143.93
65	1529	C2	NAG	366	27.879	34.326	48.881 50.081	1.00	149.17
	1530	N2	NAG	366	28.118	32.897	50.186	1.00 1.00	149.17
	1531	C7	NAG	366	28.345	32.346	51.378	1.00	149.17 149.17
	1532	07	NAG	366	28.482	33.013	52.407	1.00	149.17
70	1533 1534	ය ය	NAG	366	28.441	30.828	51.448	1.00	149.17
, 0	1004	w	. NAG	366	26. 372	34.552	49.949	1.00	149.17

	1535	03	NAG	366	25.761	34.256	51.198	1.00	149.17
	1536	C4	NAG	366	25.976	35.987	49.514	1.00	149.17
	1537	O4 ·	NAG	366	24.660	35.921	48.921	1.00	149.17
_	1538	C5	NAG	366	26.928	36.592	48,459	1.00	149.17
5	1539	Q5	NAG	366	28.320	36.323	48.766	1.00	149.17
	1540	C6	NAG	366	26.769	38,111	48.368	1.00	149.17
	1541	O 6	NAG	366	27.829	38.807	49.016	1.00	
	1542	C1	NAG	367	23.729	36.910	49.196	1.00	149.17
	1543	C2	NAG	367	22.797	37.075	47.975	1.00	173.80
10	1544	N2	NAG	367	23.536	37.637	46.860		173.80
	1545	C7	NAG	367	23.834	36.896	45.796	1.00	173.80
	1546	07	NAG	367	23.531	35.706	45.691	1.00	173.80
	1547	C8	NAG	367	24.586	37.593	44.674	1.00	173.80
	1548	C3	NAG	367	21.617	37.991		1.00	173.80
15	1549	03	NAG	367	20.711	38.025	48.311	1.00	173.80
	1550	C4	NAG	367	20.717		47.218	1.00	173.80
	1551	04	NAG	367	19.890	37.499	49.566	1.00	173.80
	1552	C5	NAG	367		38.438	49.924	1.00	173.80
	1553	O5	NAG		21.917	37.360	50.705	1.00	173.80
20	1554	C6	NAG	367	22.977	36.460	50.326	1.00	173.80
20	1555	06		367	21.347	36.810	51. 995	1.00	173.80
	1000	00	NAG	367	22.385	36.606	52. 94 8	1.00	173.80

Table 9. PhFc ϵ RI α_{1-172} , Form T1, residue exposure

>>> coordinate set= pent63_8c1.pdb

	segid	resid	resname	access	access-main	access-side
	CCCC	4	LYS	22.3151	10.9559	31.4026
5	CCCC	5	PRO	1.1153	1.4307	0.6949
	CCCC	6	LYS	16.7221	1.1596	29.1721
	CCCC	7	VAL	1.5573	2.7252	0.0000
	CCCC	8	SER	8.9731	1.8795	23.1603
	CCCC	9	LEU	3.7370	4.7824	2.6917
10	CCCC	10	ASN	12.6673	0.9406	24.3940
	CCCC	11	PRO	8.2815	0.5829	18.5464
	CCCC	12	PRO	9.7742	2.0935	20.0152
	CCCC	13	TRP	1.5926	0.1230	2.1805
	CCCC	14	ASN	3.3766	0.2934	6.4597
15	CCCC	15	ARG	1.6352	0.0000	2.5696
	CCCC	16	ILE	1.1737	0.0003	2.3470
	CCCC	17	PHE	0.2696	0.0000	0.4237
	CCCC	18	LYS	8.1283	3.2126	12.0608
	CCCC	19	GLY	5.5800	5.5800	0.0000
20	CCCC	20	GLU	3.3428	0.0000	6.0170
	CCCC	21	ASN	5.3342	3.9503 ·	6.71 82
	CCCC	22	VAL	0.3267	0.4564	0.1538
	CCCC	23	THR	5.3278	0.0157	12.4107
	CCCC	24	LEU	0.2562	0.0002	0.5121
25	CCCC	25	THR	4.7853	0.0002	11.1657
	CCCC	26	CYS	0.2343	0.3249	0.0530
	CCCC	27	ASN	7.7637	1.8546	13.6728
	CCCC	28	GLY	7.9103	7.9103	0.0000
	CCCC	29	ASN	16.6538	7.7758	25.5318
30	CCCC	30	ASN	14.2106	9.9392	18.4821
	CCCC	31	PHE	18.4293	8.6833	23.9984
	CCCC	32	PHE	6.9543	6.9847	6.9370
	CCCC	33	GLU	17.3275	4.6057	27.5049
	CCCC	34	VAL	9.7070	3.0781	18.5455
35	CCCC	35	SER	14.3512	2.1631	38.7274
	CCCC	36	SER	7.0113	1.9003	17.2334
	CCCC	37	THR	0.7139	1.2493	0.0000
	CCCC	38	LYS	8.3149	0.3194	14.7113
	CCCC	39	TRP	0.0064	0.0013	0.0084
40	CCCC	40	THE	3.0089	0.0000	4.7283
	CCCC	41	HIS	3.3635	0.3462	5.3750
	CCCC	42	ASN	5.9924	6.1741	5.8107
	CCCC	43	GLY	8.7956	8.7956	0.0000
	CCCC	44	SER	10.0868	2.4356	25.3890
45	CCCC	45	LEU	14.4496	6.7421	22.1571
	CCCC	46	SER	4.8664	3.2655	8.0682
	CCCC	47	GLU	13.8158	4.4486	21.3095
	CCCC	48	GLU	3.7957	0.7742	6.2129
	CCCC	49	THR	11.0308	0.0826	25.6285
50	CCCC	50	ASN	3.7680	0.9608	6.5753
_ -	CCCC	51	SER	0.9943	0.0001	2.9826
				0.0070	0.0001	2.3020

	CCCC	52 53 54	SER - LEU ASN	2.8849 2.6956	0.0003 0.0208	8.6541 5.3704
	CCCC	5 4 55	ILE	7.0487	3.7820	10.3153
5	CCCC	56	VAL	2.0484 8.3718	1.5241	2.5727
•	CCCC	57	ASN	6.8809	1.8780 0.9872	17.0302
	CCCC	58	ALA	0.3689	0.9872 0.4454	12.7747
	CCCC	59	LYS	8.8541	0.4454	0.0628
	CCCC	60	PHE	3.1986	0.2109	15.9126
10	CCCC	61	GLU	8.5928	0.1580	4.9058 15.3407
	CCCC	62	ASP	4.2001	0.0802	8.3200
	CCCC	63	SER	0.1586	0.0002	0.4759
	CCCC	64	GLY	0.0205	0.0205	0.0000
	CCCC	65	GLU	3.1362	0.1046	5.5614
15	CCCC	66	TYR	0.7765	0.0000	1.1648
	CCCC	67	LYS	3.3029	0.0005	5.9449
	CCCC	68	CYS	0.0000	0.0000	0.0000
	CCCC	69	GLN	3.8782	0.0000	6.9808
	CCCC	70	HIS	2.2973	0.2891	3.6361
20	CCCC	71	GLN	15.5567	6.4047	22.8783
	CCCC	72	GLN	18.9536	6.5187	28.9015
	CCCC	73	VAL	6.3773	2.6597	11.3340
•	CCCC	74	ASN	7.2490	0.8511	13.6469
	CCCC	75	GLU	9.5776	4.4490	13.6806
25	CCCC	76	SER	0.7222	1.0831.	0.0006
	CCCC	77	GLU	13.3681	1.0686	23.2077
	CCCC	78	PRO	2.7891	1.9776	3.8710
	CCCC	79	VAL	5.1775	0.7766	11.0455
	CCCC	80	TYR	3.7512	1.4544	4.8996
30	CCCC	81	LEU	0.2610	0.0000	0.5221
	CCCC	82	GLU	5.7107	0.0011	10.2784
	CCCC	83	VAL	1.5280	2.6739	0.0000
	CCCC	84	PHE	2.6808	0.7184	3.8022
25	CCCC	85	SER	5.8 78 7	5.8008	6.0345
35	CECC	86	ASP	6.0903	2.6973	9.4832
	CCCC	87	TRP	3.0930	0.2603	4.2261
	CCCC	88	LEU	0.0403	0.0675	0.0131
	CCCC	89	LEU	0.1021	0.0000	0.2041
40	CCCC	90	LEU	0.0000	0.0000	0.0000
40	CCCC	91	GLN	0.2597	0.0000	0.4674
	CCCC	92	ALA	0.0596	0.0563	0.0730
	CCCC	93	SER	4.6788	3.0077	8.0211
	CCCC	94	ALA	8.5911	1.3052	37.7350
45	CCCC	95	GLU	4.4767	1.5831	6.7916
40	CCCC	96	VAL	4.3906	4.6557	4.0371
	CCCC	97	VAL	1.4394	1.1406	1.8378
	CCCC	98 99	MET GLU	13.6889	0.2044	27.1734
	CCCC	100	GLY	7.4797	4.8677	9.5692
50	CCCC	101	GLN	5.3567	5.3567	0.0000
50	CCCC	102	PRO	9.7722	0.0006	17.5894
	CCCC	103	LEU	9.4569	1.5764	19.9642
	CCCC	103	PHE	0.0179 6.2358	0.0357	0.0000
	CCCC	105	LEU	6.2358	0.0000	9.7991
55	CCCC	106	ARG	0.0474 2.3314	0.0488	0.0461
	CCCC	107	CYS	0.7781	0.0000	3.6636
		,	0.0	. 0.7701	1.1549	0.0246

	CCCC	108	HIS	1.2171	0.3012	1.8277
	CCCC	109	GLY	1.2651	1.2651	0.0000
	CCCC	110	TRP	1.9508	0.3094	2.6074
	CCCC	111	ARG	7.1821	6.7612	7.4226
5	CCCC	112	ASN	12.7243	3.8235	21.6251
3	CCCC	113	TRP	2.9331	3.2961	2.7878
	CCCC	114	ASP	11.7314	2.0501	21.4128
	CCCC	115	VAL	0.8918	0.6165	1.2589
	CCCC	116	TYR	5.7191	0.0000	8.5787
10	CCCC	117	LYS	10.9908	0.9471	19.0258
10	CCCC	118	VAL	0.0001	0.0000	0.0002
	CCCC	119	ILE	4.7127	0.0007	9.4248
	CCCC	120	TYR	0.0060	0.0000	0.0091
	CCCC	121	TYR	3.6424	0.0150	5.4562
15	CCCC	122	LYS	3,9385	0.8428	6.4150
15	CCCC	123	ASP	11.0597	7.2355	14.8840
	CCCC	124	GLY	13.5829	13.5829	0.0000
	CCCC	125	GLU	13.1544	0.5211	23.2611
	CCCC	126	ALA	15.0490	5.4493	53.4477
20	CCCC	127	LEU	9.4150	6.1124	12.7176
20	CCCC	128	LYS	11.5717	1.7494	19.4295
	CCCC	129	TYR	10.5011	5.5905	12.9565
	CCCC	130	TRP	8.0873	0.9625	10.9373
	CCCC	131	TYR	11.7870	1.0734	17.1438
25	CCCC	132	GLU	12.6705	2.2279.	21.0247
25	CCCC	133	ASN	5.3027	5.3599	5.2454
	CCCC	134	HIS	8.2476	1.2608	12.9055
	CCCC	135	ASN	1.2965	0.3213	2.2717
	CCCC	136	ILE	2.0165	1.3778	2.6552
20	CCCC	137	SER	9.9968	7.2656	15.4593
30	CCCC	138	ILE	3.6077	0.9873	6.2280
	CCCC	139	THR	15.8360	2.4317	33.7085
	CCCC	140	ASN	6.0823	3.6720	8.4926
	CCCC	141	ALA	0.0000	0.0000	0.0000
35	CCCC	142	THR	6.7820	0.1381	15.6405
55	CCCC	143	VAL	5.0630	1.4175	9.9237
	CCCC	144	GLU	14.1160	4.3532	21.9263
	CCCC	145	ASP	4.3317	0.0259	8.6374
	CCCC	146	SER	5.1283	3.0010	9.3829
40	CCCC	147	GLY	3.4210	3.4210	0.0000
40	CCCC	148	THR	5.2803	0.0914	12.1988
	CCCC	149	TYR	0.2014	0.0000	0.3021
	CCCC	150	TYR	3.7574	0.0000	5.6362
	CCCC	151	CYS	0.0001	0.0001	0.0000
45	CCCC	152	THR	3.8919	0.0107	9.0668
43	CCCC	153	GLY	1.0188	1.0188	0.0000
	CCCC	154	LYS	6.4238	0.0528	11.5207
	CCCC	155	VAL	0.4180	0.0000	0.9754
	CCCC	156	TRP	3.3279	3.7718	3.1504
50	CCCC	157	GLN	13.1268	3.2479	21.0299
30	CCCC	158	LEU	8.7018	0.1257	17.2778
	CCCC	159	ASP	14.2676	4.9595	23.5758
	CCCC	160	TYR	2.2687	2.5573	2.1243
	CCCC	161	GLU	12.1767	4.4230	18.3798
55	CCCC	162	SER	1.1841	1.7762	0.0000
55	CCCC	163	GLU	9.4913	0.1747	16.9445

				•		
	CCCC	164	PRO	9.7765	1.5124	20.7953
	CCCC	165	LEU	1.6495	0.1289	3.1701
	CCCC	166	ASN	3.4007	0.7824	6.0190
	CCCC	167	ILE	0.5293	1.0585	0.0000
5	CCCC	168	THR	3.2321	0.0380	7.4909
3	CCCC	169	VAL	0.0723	0.1266	0.0000
	CCCC	170	ILE	2.2951	0.0689	4.5213
	CCCC	171	LYS	14.3432	12.9256	15.4773
		221	NAG	11.7001	0.0000	11.7001
10	CCCC	222	NAG	14.4010	0.0000	14.4010
10	CCCC		NAG	7.1046	0.0000	7.1046
	CCCC	242	NAG	8.0078	0.0000	8.0078
	CCCC	243		16.5438	0.0000	16.5438
	CCCC	244	MAN		0.0000	16.2147
	cccc	250	NAG	16.2147	0.0000	21.7742
15	CCCC	274	NAG	21.7742	0.0000	15.0979
	CCCC	335	NAG	15.0979	0.0000	17.6065
	CCCC	340	NAG	17.6065		11.8776
	CCCC	366	NAG	11.8776	0.0000	19.0810
	CCCC	367	NAG	19.0810	0.0000	
20	AAAA	4	LYS	15.9363	6.7194	23.3099
	AAAA	5	PRO	1.1488	1.4481	0.7498
	AAAA	6	LYS	13.8574	1.1896	23.9916
	AAAA	7	VAL	1.5646	2.7375	0.0007
	AAAA	8	SER	9.0558	1.9390	23.2893
25	AAAA	9	LEU	3.8393	4.9388	2.7398
	AAAA	10	ASN	12.5152	0.9543	24.0762
	AAAA	11	PRO	8.3710	0.5349	18.8192
	AAAA	12	PRO	9.8889	2.0781	20.3033
	AAAA	13	TRP	1.5673	0.1143	2.1485
30	AAAA	14	ASN	3.1275	0.2808	5.9741
50	AAAA	15	ARG	1.6130	0.0057	2.5315
	AAAA	16	ILE	1.1993	0.0000	2.3986
	AAAA	17	PHE	0.2501	0.0000	0.3929
	AAAA	18	LYS	10.8021	3.4649	16.6720
35	AAAA	19	GLY	5.6 93 9	5.6939	0.0000
J J	AAAA	20	GLU	3.4960	0.0003	6.2926
	AAAA	21	ASN	5.3970	4.0391	6.7548
	AAAA	22	VAL	0.2660	0.3430	0.1633
	AAAA	23	THR	5.2134	0.0418	12.1090
40	AAAA	24	LEU	0.2554	0.0007	0.5101
40	AAAA	25	THR	4.8655	0.0005	11.3521
			CYS	0.2307	0.3194	0.0532
	AAAA	26 27	ASN	0.4259	0.2949	0.5569
	AAAA	28	GLY	4.4162	4.4162	0.0000
45			ASN	7.6150	7.1438	8.0862
45	AAAA	29	ASN	11.3939	10.0050	12.7829
	AAAA	30	PHE	14.7556	4.8219	20.4320
	AAAA	31		2.7147	4.5718	1.6536
	AAAA	32	PHE		4.4574	9.9787
	AAAA	33	GLU	7.5248	3.0519	5.4642
50	AAAA	34	VAL	4.0858		39.0790
	AAAA	35	SER	14.4683	2.1629	
	AAAA	36	SER	6.9471	1.9207	16.9999 0.0000
	AAAA	37	THR	0.7130	1.2478	
	AAAA	38	LYS	8.2623	0.2915	14.6390
55	AAAA	39	TRP	0.0071	0.0080	0.0067
	AAAA	40	PHE:	2.9948	0.0014	4.7054

	AAAA	41	HIS	3.3204	0.4762	5.2166
	AAAA	42	ASN	6.4516	7.1677	5.7356
•	AAAA	43	GLY	9.6929	9.6929	0.0000
	AAAA	44	SER	12.5467	3.0596	31.5 209
5	AAAA	45	LEU	14.0527	6.3669	21.7524
3	AAAA	46	SER	5.9554	3.7890	10.2883
	AAAA	47	GLU	19.8848	8.0231	29.3741
	AAAA	48	GLU	6.1436	2.1551	9.3344
	AAAA	49	THR	10.8974	0.0037	25.4223
10	AAAA	50	ASN	3.7283	0.9830	6.4736
10	AAAA	51	SER	1.0424	0.0007	3.1257
	AAAA	52	SER	2.9027	0.0000	8.7080
	AAAA	53	LEU	2.6315	0.0203	5.2426
	AAAA	54	ASN	7.1111	3.9443	10.2778
15	AAAA	55	ILE	2.099ఏ	1.5522	2.6464
	AAAA	56	VAL	11.4229	1.8784	24.1489
	AAAA	57	ASN	9.2772	0.9862	17.5682
	AAAA	58	ALA	0.3197	0.3981	0.0062
	AAAA	59	LYS	13.5164	0.0175	24.3155
20	AAAA	60	PHE	3.5563	0.1394	5.5088
	AAAA	61	GLU	8.5716	0.1791	15.2857
	AAAA	62	ASP	4.2001	0.0591	8.3412
	AAAA	63	SER	0.1501	0.0000	0.4504
	AAAA	64	GLY	0.0335	. 0.0335	0.0000
25	AAAA	65	GLU	8.1768	0.0971 .	14.6406
	AAAA	66	TYR	0.7839	0.0002	1.1758
	AAAA	67	LYS	3.2196	0.0004	5.7951
	AAAA	68	CYS	0.0000	0.0000	0.0000
	AAAA	69	GLN	3.8577	0.0000	6.9439
30	AAAA	70	HIS	0.2845	0.2473	0.3093
	AAAA	71	GLN	14.8691	6.1965	21.8072
	AAAA	72	GLN	18.3340	6.2079	28.0348
	AAAA	73	VAL	3.2302	2.5357	4.1564
	AAAA	74	ASN	7.3440	0.8492	13.8389
35	AAAA	75	GLU	9.5554	4,4097	13.6718
	AAAA	76	SER	0.5321	0.7981	0.0000 28.1176
	AAAA	77	GLU	16.0334	0.9282	
	AAAA	78	PRO	8.2987	5.2204	12.4031 12.0789
	AAAA	79	VAL	5.9326	1.3229	9.1664
40	AAAA	80	TYR	6.7460	1.9053	0.5469
	AAAA	81	LEU	0.2734	0.0000	10.3651
	AAAA	82	GLU	5.7587	0.0007 2.6843	0.0000
	AAAA	83	VAL	1.5339		3.9361
	AAAA	84	PHE	2.7544	0.6865 5.9578	21.4274
45	AAAA	85	SER	11.1143	2.2574	9.9474
	AAAA	86	ASP	6.1024	0.2983	12.7613
	AAAA	87	TRP	9.2004	0.2963	0.0051
	AAAA	88	LEU	0.0297	0.0000	0.1854
50	AAAA	89	LEU	0.0927	0.0000	0.0002
50	AAAA	90	LEU	0.0001 0.2535	0.0000	0.4563
	AAAA	91	GLN		0.0000	0.0344
	AAAA	92	ALA	0.0453 4.6084	2.9327	7.9597
	AAAA	93	SER		1.2990	38.3529
	AAAA	94	ALA GLU	8.7098 7.3017	1.5643	11.8916
55	AAAA	95		12.9692	4.7889	23.8762
	AAAA	96	VAL ·	12.3032	7.7003	_5.57 52

	AAAA	97	VAL	1.4036	1.0908	1.8207
	AAAA	98	MET	7.3760	0.2425	14.5094
	AAAA	99	GLU	7.1208	4.6443	9.1019
	AAAA	100	GLY	5.2380	5.2380	0.0000
5	AAAA	101	GLN	3.2910	0.0195	5.9082
J	AAAA	102	PRO	5.1174	1.6052	9.8002
	AAAA	103	LEU	0.0323	0.0600	0.0045
	AAAA	104	PHE	6.3337	0.0009	9.9525
	AAAA	105	LEU	0.0742	0.0597	0.0887
10	AAAA	106	ARG	2.3217	0.0000	3.6484
10	AAAA	107	CYS	0.7916	1.1873	0.0000
	AAAA	108	HIS	1.2205	0.3014	1.8333
	AAAA	109	GLY	1.3688	1.3688	0.0000
	AAAA	110	TRP	4.3961	0.3129	6.0293
15	AAAA	111	ARG	14.1659	6.8259	18.3603
13	AAAA	112	ASN	12.3349	3.8047	20.8651
	AAAA	113	TRP	7.3124	3.4188	8.8699
	AAAA	114	ASP	11.5788	1.5704	21.5873
	AAAA	115	VAL	0.8933	0.6941	1.1589
20	AAAA	116	TYR	5.1843	0.0006	7.7761
20	AAAA	117	LYS	7.1256	0.9679	12.0517
	AAAA	118	VAL	0.0000	0.0000	0.0000
	AAAA	119	ILE	1.4302	0.0000	2.8604
	AAAA	120	TYR	0.0104	0.0005	0.0153
25	AAAA	121	TYR	2.8600	0.0167.	4.2816
	AAAA	122	LYS	3.8739	0.7828	6.3468
	AAAA	123	ASP	11.0893	7.0588	15.1198
	AAAA	124	GLY	13.7649	13.7649	0.0000
	AAAA	125	GLU	8.1492	0.5254	14.2483
30	AAAA	126	ALA	1.3596	0.7744	3.7005
50	AAAA	127	LEU	5.0008	0.9822	9.0194
	AAAA	128	LYS	10.8601	0.1501	19.4280
	AAAA	129	TYR	5.7014	3.8333	6.6354
	AAAA	130	TRP	7.7631	0.9621	10.4835
35	AAAA	131	TYR	3.0458	1.1141	4.0116
	AAAA	132	GLU	11.1091	2.1808	18.2518
	AAAA	133	ASN	5.2028	5.3196	5.0859
	AAAA	134	HIS	8.3482	1.2156	13.1032
	AAAA	135	ASN	1.2934	0.3190	2.2679
40	AAAA	136	ILE	2.1274	1.3695	2.8853
	AAAA	137	SER	10.0348	7.2335	15.6375
	AAAA	138	ILE	3.6211	1.0099	6.2322
	AAAA	139	THR	16.0640	2.580პ	34.0420
	AAAA	140	ASN	5.4194	3.6273	7.2114
45	AAAA	141	ALA	0.0000	0.0000	0.0000
	AAAA	142	THR	7.2278	0.4616	16.2495
	AAAA	143	VAL	7.6811	1.4982	15.9250
	AAAA	144	GLU	14.2939	4.1689	22.3939
	AAAA	145	ASP	4.3509	0.0318	8.6701
50	AAAA	146	SER	5.2566	3.1044	9.5609
	AAAA	147	GLY	3.2376	3.2376	0.0000
	AAAA	148	THR	5.2658	0.0995	12.1542
	AAAA	149	TYR	0.2165	0.0000	0.3248
	AAAA	150	TYR	3.8830	0.0000	5.8245
55	AAAA	151	CYS	0.0000	0.0000	0.0000
	AAAA	152	THR	3.7398	0.0010	8.7248

	AAAA	153	GLY	1.0201	1.0201	0.0000
	AAAA	154	LYS	4.0119	0.0425	7.1873
	AAAA	155	VAL	0.4567	0.0000	1.0656
	AAAA	156	TRP	11.1226	3.7204	14.0834
5	AAAA	157	GLN	8.2831	3.3029	12.2673
)	AAAA	158	LEU	13.8927	0.1434	27.6420
	AAAA	159	ASP	9.7733	4.0346	15.5120
	AAAA	160	TYR	3.4354	2.0054	4.1504
	AAAA	161	GLU	8.2007	5.4400	10.4093
10			SER	1.2173	1.8259	0.0002
10	AAAA	162	GLU	9,4751	0.3080	16.8088
	AAAA	163	PRO	9.8187	1.5247	20.8774
	AAAA	164		1.6583	0.0972	3.2194
	AAAA	165	LEU	4.2239	1.2362	7.2117
	AAAA	166	ASN	0.5672	1.1307	0.0038
15	AAAA	167-	ILE		0.0604	21.7538
	AAAA	168	THR	9.3576		0.0074
	AAAA	169	VAL	0.5466	0.9510	19.7663
	AAAA	170	ILE	10.6664	1.5666	24.4247
	AAAA	171	LYS	20.0709	14.6286	
20	AAAA	221	NAG	13.0731	0.0000	13.0731
	AAAA	222	NAG	19.9260	0.0000	19.9260
	AAAA	242	NAG	10.0968	0.0000	10.0968
	AAAA	243	NAG	9.7429	0.0000	9.7429
	AAAA	244	MAN	16.5025	0.0000	16.5025
25	AAAA	250	NAG	16.0048	0.0000 -	16.0048
	AAAA	274	NAG	21.9758	0.0000	21.9758
	AAAA	335	NAG	15.0266	0.0000	15.0266
	AAAA	340	NAG	10.2058	0.0000	10.2058
	AAAA	366	NAG	14.2003	0.0000	14.2003
30	AAAA	367	NAG	21.1043	0.0000	21.1043
	BBBB	4	LYS	21.2711	8.1950	31.7320
	BBBB	5	PRO	0.9327	1.4134	0.2918
	BBBB	6	LYS	13.5721	0.9858	23.6411
	BBBB	7	VAL	1.5696	2.7468	0.0000
35	BBBB	8	SER	9.0540	1.8158	23.5305
	BBBB	9	LEU	3.7548	4.6164	2.8932
	BBBB	10	ASN	12.3838	0.9742	23.7933
	BBBB	11	PRO	8.3839	0.5771	18.7929
	BBBB	12	PRO	10.2255	2.2114	20.9110
40	BBBB	13	TRP	1.5767	0.1420	2.1505
	BBBB	14	ASN	3.6856	0.2734	7.0977
	BBBB	15	ARG	1.6517	0.0084	2.5908
	BBBB	16	ILE	1.1539	0.0000	2.3079
	BBBB	17	PHE	0.2627	0.0000	0.4128
45	BBBB	18	LYS	10.5872	3.1464	16.5399
	BBBB	19	GLY	5.2452	5.2452	0.0000
	BBBB	20	GLU	3.4004	0.0000	6.1208
	BBBB	21	ASN	5.3165	3.8893	6.7437
	BBBB	22	VAL	0.3290	0.4639	0.1492
50	BBBB	23	THR	5.3376	0.0419	12.3986
	BBBB	24	LEU	0.2556	0.0000	0.5112
	BBBB	25	THR	4.8687	0.0000	11.3603
	8888	26	CYS	0.2112	0.2986	0.0364
	BBBB	27	ASN	0.5141	0.1099	0.9184
55	BBBB	28	GLY	2.2181	2.2181	0.0000
	BBBB	29	ASN	10.0991	5.9026	14.2956

	BBBB	30	ASN	8,2629	8.5326	7.9932
	BBBB	31	PHE	13.1098	3.1872	18.7798
	BBBB	32	PHE	3.2118	5.7094	1.7846
	BBBB	33	GLU	9.8599	4.6157	14.0553
5	BBBB	34	VAL	4.2409	3.1111	5.7472
J	BBBB	35	SER	14.4622	2.1340	39.1186
	BBBB	36	SER	7.0903	1.9980	17.2748
	BBBB	37	THR	0.7246	1.2681	0.0000
	BBBB	38	LYS	8.3435	0.2936	14.7834
10	8888	39	TRP	0.0045	0.0000	0.0063
10	8888	40	PHE	3.0307	0.0013	4.7618
	BBBB	41	HIS	3.2985	0.2952	5.3007
	BBBB	42	ASN	3.9446	4.4215	3.4677
	BBBB	43	GLY	6.4 44 8	6.4448	0.0000
15	BBBB	44	SER	7.9300	1.5277	20.7347
13	8888	45	LEU	14.0360	6.3402	21.7318
	BBBB	46	SER	5.3085	3.4386	9.0482
	BBBB	47	GLU	19.8137	7.9994	29.2651
•	8888	48	GLU	6.1811	2.3816	9.2207
20	BBBB	49	THR	10.8045	0.0111	25.1957
20	BBBB	50	ASN	3.7967	1.0050	6.5885
	BBBB	51	SER	1.0119	0.0000	3.0357
	BBBB	52	SER	2.8985	0.0010	8.6934
	BBBB	53	LEU	2.8664	0.0001	5.7327
25	BBBB	54	ASN	7.0968	3.9693	10.2244
20.	BBBB	55	ILE	2.0503	1.4906	2.6099
	BBBB	56	VAL	11.3539	1.8189	24.0671
	BBBB	57	ASN	9.2620	1.0325	17.4916
	BBBB	58	. ALA	0.3961	0.4951	0.0000
30	BBBB	59	LYS	13.4689	0.0284	24.2213
•	BBBB	60	PHE	3.3978	0.2767	5.1813
	BBBB	61	GLU	8.8117	0.1782	15.7185
	BBBB	62	ASP	4.1350	0.0756	8.1943
	BBBB	63	SER	0.1730	0.0000	0.5191
35	BBBB	64	GLY	0.0000	0.0000	0.0000
	BBBB	65	GLU	6.5484	0.0001	11.7871
	BBBB	66	TYR	0.7915	0.0000	1.1872
	BBBB	67	LYS	3.2805	0.0000	5.9049
	BBBB	68	CYS	0.0000	0.0000	0.0000
40	BBBB	69	GLN	3.8141	0.0000	6.8654
	88 8 8	70	HIS	0.1609	0.2608	0.0943
	BBBB	71	GLN	10.6127	5.2959	14.8662 10.3096
	BBBB	72	GLN	8.4010	6.0152	
	BBBB	73	VAL	2.9562	2.5768	3.4619
45	BBBB	74	ASN	7.3147	0.9982	13.6312
	BBBB	75	GLU	9.4113	4.1701	13.6043
	BBBB	76	SER	0.5684	0.8526	0.00 00 27.7 278
	BBBB	77	GLU	15.8600	1.0254	
	8888	78	PRO	8.2998	5.0247	12.6666
50	BBBB	79	VAL	5.5759	1.3782	11.1729 8.3734
	BBBB	80	TYR	6.2317	1.9484	0.4975
	8888	81	LEU	0.2490	0.0005	
	BBBB	82	GLU	5.8300	0.0000	10.4940 0.0000
	BBBB	83	VAL	1.5904	2.7832	3.8756
55	BBBB	84	PHE	2.7220	0.7033	20.527
	BBBB	85	SER	10.7069	5.7965	20.321.

	BBBB	86	ASP	5.9874	2.1888	9.7860
_	BBBB	87	TRP	9.1171	0.3262	12.6335
	BBBB	88	LEU	0.0289	0.0578	0.0000
_	BBBB	89	LEU LEU	0.0888 0.0000	0.0000 0.0000	0.1776 0.0000
5	BBBB	90 91	GLN	0.2626	0.0000	0.4726
	BBBB	92	ALA	0.2626	0.0399	0.4726
	BBBB		SER	4.6672	2.9572	8.0872
	BBBB	93 94	ALA	8.7256	1.3164	38.3623
10	BBBB	9 4 95	GLU	7.1 764	1.5358	11.6889
10	BBBB	96	VAL	12.6418	4.7054	23.2237
	BBBB		VAL	1.4061	1.1339	1.7691
	BBBB	97		11.9430	0.2070	23.6789
	BBBB	98	MET GLU	7.2607	4.6466	9.3520
1.5	BBBB	99 100	GLY	5.1244	5.12 44	0.0000
15	BBBB	100	GLY	4.0221	0.0000	7.2398
	BBBB BBBB	101	PRO	7.3498	1.5529	15.0790
		102	LEU	0.0071	0.0138	0.0004
	BBBB BBBB	103	PHE	6.2937	0.0007	9.8898
20	BBBB	105	LEU	0.0567	0.0603	0.0531
20	BBBB	106	ARG	2.3037	0.0000	3.6201
	BBBB	107	CYS	0.8127	1.2098	0.0186
	BBBB	107	HIS	1.1982	0.2627	1.8218
	BBBB	109	GLY	1.2842	1.2842	0.0000
25	888B	110	TRP	4.4804	0.3255	6.1423
23	8888	111	ARG	14.4479	6.9241	18.7472
	BBBB	112	ASN	12.2860	3.9115	20.6605
	888B	113	TRP	7.0297	3.4023	8.4806
	BBBB	114	ASP	11.5554	1.8648	21.2461
30	BBBB	115	VAL	0.8700	0.6238	1.1983
30	BBBB	116	TYR	5.8899	0.0000	8.8349
	8888	117	LYS	11.0072	0.9540	19.0498
	BBBB	118	VAL	0.0000	0.0000	0.0000
	BBBB	119	ILE	4.7824	0.0000	9.5649
35	BBBB	120	TYR	0.0292	0.0003	0.0436
23	BBBB	121	TYR	3.6258	0.0127	5.4323
	BBBB	122	LYS	3.8173	0.8234	6.2125
	BBBB	123	ASP	11.1350	7.1239	15.1460
	8888	124	GLY	13.9353	13.9353	0.0000
40	8888	125	GLU	13.4298	0.5494	23.7341
40	8888	126	ALA .	15.0233	5.4413	53.3510
	BBBB	127	LEU	9.2699	5.9635	12.5762
	8888	128	LYS	11.6633	1.8096	19.5508
	8888	129	TYR	10.3608	5.2815	12.9005
45	BBBB	130	TRP	8.0170	1.0064	10.8213
-1.5	8888	131	TYR	11.7311	1.0656	17.0638
	BBBB	132	GLU	12.8760	2.2402	21.3846
	8888	133	ASN	5.2983	5.3131	5.2835
	BBBB	134	HIS	7.9203	1.2177	12.3886
50	BBBB	135	ASN	1.3098	0.3200	2.2995
50	BBBB	136	ILE	2.0145	1.4037	2.6254
	BBBB	137	SER	9.9370	7.1329	15.5453
	BBBB	138	ILE	3.5989	0.9814	6.2165
	BBBB	139	THR	16.3957	2.4548	34.9836
55	BBBB	140	ASN	6.1076	3.6820	8.5333
	BBBB	141	ALA	0.0000	0.0000	0.0000

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	888B 888B	142 143	THR VAL	6.9409 8.0179	0.3571 1.4651	15.7193
	BBBB	144	GLU	13.9749	4.2931	16.7550 21.7203
	8888	145	ASP	4.2546	0.0236	8.4857
5	BBBB	146	SER	5,2200	3.1447	9.3705
•	BBBB	147	GLY	3.2638	3.2638	0.0000
	8888	148	THR	5.2033	0.0855	12.0270
	8888	149	TYR	0.2349	0.0000	0.3523
	BBBB	150	TYR	3.8297	0.0006	5.7443
10	BBBB	151	CYS	0.0001	0.0002	0.0000
	BBBB	152	THR	3.8729	0.01 15	9.0216
	BBBB	153	GLY	1.0080	1.0080	0.0000
	BBBB	154	LYS	6.2899	0.0456	11.2854
	BBBB	155	VAL	0.4338	0.0000	1.0121
15	BBBB	156	TRP	10.7002	3.5331	13.6790
	8888	157	GLN	13.5388	3.3217	21.7125
	BBBB	158	LEU	13.7581	0.1277	27.3885
	BBBB	159	ASP	13.8236	4.9295	22.7177
20	8888	160	TYR	3.3842	2.5049	3.8239
20	8888 8888	161	GLU	12.8172	5.3317	18.8056
		162	SER	1.1166	1.6744	0.0011
	8888 8888	163 164	GLU PRO	9.2415	0.1789	16.4915
	BBBB	165	LEU	9.7119	1.5204	20.6339
25	8888	166	ASN	1.6353 4.1241	0.0985 1.1171 -	3.1722
2,5	8888	167	ILE	0.5678	1.1351	7.1311 0.0006
	BBBB	168	THR	9.4957	0.0238	22.1247
	BBBB	169	VAL	0.5214	0.9124	0.0000
	BBBB	170	ILE	10.7674	1.5460	19.9889
30	BBBB	171	LYS	19.3575	14.1022	23.5617
	BBBB	221	NAG	13.1653	0.0000	13.1653
	BBBB	222	NAG	20.0638	0.0000	20.0638
	BBBB	242	NAG	5.8770	0.0000	5.8770
	BBBB	243	NAG	6.5918	0.0000	6.5918
35	BBBB	244	MAN	16.4886	0.0000	16.4886
	BBBB	250	NAG	16.1285	0.0000	16.1285
	BBBB	274	NAG	20.2170	0.0000	20.2170
	BBBB	335	NAG	14.9859	0.0000	14.9859
40	BBBB	340	NAG	17.5037	0.0000	17.5037
40	BBBB	366	NAG	14.5337	0.0000	14.5337
	BBBB	367	NAG	21.0686	0.0000	21.0686
	DDDD	4	LYS	22.4057	10.8330	31.6640
		5	PRO	1.1546	1.4746	0.7280
45	DDDD	6 7	LYS VAL	17.0122	1.1737	29.6830
7.7	DDDD	8	SER	1.5813 9.0050	2.7670	0.0004
	DDDD	9	LEU	3.6933	1.8942 4.6049	23.2265
	DDDD	10	ASN	12.3091	1.0020	2.7818 23.6161
	DDDD	11	PRO	8.3171	0.5504	18.6727
50	DDDD	12	PRO	9.9864	2.1032	20.4973
	DDDD	13	TRP	1.5517	0.0931	2.1352
	DDDD	14	ASN	3.3780	0.3110	6.4451
	DDDD	15	ARG	1.6343	0.0116	2.5615
	DDDD	16	ILE	1.1547	0.0005	2.3088
55	DDDD	17	PHE	0.2492	0.0000	0.3916
	סססס	18	LYS	4.6732	2.0544	6.7683
					•	

	DDDD	19	GLY	3.1162	3.1162	0.0000
	DDDD	20	GLU	3.5200	0.0000	6.3359
	DDDD	21	ASN	5.4287	3.8849	6.9725
	DDDD	22	VAL	0.3155	0.4412	0.1479
5	DDDD	23	THR	5.1394	0.0324	11.9489
Τ,	DDDD	24	LEU	0.2366	0.0000	0.4733
	DDDD	25	THR	4.8738	0.0000	11.3721
	DDDD	26	CYS	0.2520	0.3402	0.0757
	DDDD	27	ASN	7.6624	1.9816	13.3432
10	DDDD	28	GLY	7.7316	7.7316	0.0000
	DDDD	29	ASN	17.3095	8.4320	26.1871
	DDDD	30	ASN	14.6001	10.1471	19.0532
	DDDD	31	PHE	18.5570	8.7657	24.1521
	DDDD	32	PHE	7.0815	6.8006	7.2420
15	DDDD	33	GLU	17.2171	4.7180	27.2164
	DDDD	34	VAL	10.0324	3.1007	19.2746
	DDDD	35	SER	14.2871	2.1039	38.6536
	DDDD	36	SER	6.9328	1.7803	17.2376
	DDDD	37	THR	0.7026	1.2295	0.0000
20	DDDD	38	LYS	8.3451	0.3160	14.7683
	DDDD	39	TRP	0.0041	0.0023	0.0049
	DDDD	40	PHE	2.9900	0.0009	4.6980
	DDDD	41	HIS	3.3768	0.3997	5.3616
	DDDD	42	ASN	6.4948	7.0880	5.9016
25	DDDD	43	GLY	9.5817	9.5817 ·	0.0000
	DDDD	44	SER	12.6350	2.9429	32.0194
	DDDD	45	LEU	14.2578	6.4935	22.0220
	DDDD	46	SER	5.6757	3.8029	9.4212
	DDDD	47	GLU	19.9087	7.8667	29.5 423
30	DDDD	48	GLU	6.0890	2.3899	9.0482
	DDDD	49	THR	10.8314	0.0116	25.2577
	DDDD	50	ASN	3.8373	0.9946	6.6800
	DDDD	51	SER	0.9841	0.0000	2.9524
	DDDD	52	SER	2.8765	0.0001	8.6293
35	DDDD	53	LEU	2.8376	0.0187	5.6565
	DDDD	54	ASN	7.0382	3.8726	10.2037
	DDDD	55	ILE	2.0467	1.4442	2.6492
•	DDDD	56	VAL	11.5050	1.8629	24.3611
	DDDD	57	ASN	8.8180	1.0298	16.6062
40	DDDD	58	ALA	0.2350	0.2934	0.0018
	DDDD	59	LYS	13.6844	0.0264	24.6108
	DDDD	60	PHE	2.6066	0.0006	4.0957
	DDDD	61	GLU	8.6110	0.1659	15.3671
	DDDD	62	ASP	4.2057	0.0884	8.3230
45	DDDD	63	SER	0.1340	0.0000	0.4019
	DDDD	64	GLY	0.0349	0.0349	0.0000
	DDDD	65	GLU	8.1888	0.0852	14.6716
	DDDD	66	TYR	0.7677	0.0000	1.1516
	DDDD	67	LYS	3.2893	0.0000	5.9208
50	DDDD	68	CYS	0.0005	0.0000	0.0014
	DDDD	69	GLN	3.8578	0.0000	6.9441
	DDDD	70	HIS	2.2626	0.2237	3.6218
	DDDD	71	GLN	15.3304	6.1240	22.6955
	DDDD	72	GLN	18.9257	6.3446	28.9906
55	DDDD	73	VAL	6.4935	2.6517	11.6159
	DDDD	74	ASN	7.2861	0.8315	13.7407

	DDDD	75	GLU	9.5469	4.3906	13.6720
	DDDD	76	SER	0.4742	0.7107	0.0011
	DDDD	77	GLU	16.0719	0.9787	28.1465
	DDDD	78	PRO	8.1673	5.2859	12.0091
5	DDDD	79	VAL	5.7531	1.2596	11.7443
J	DDDD	80	TYR	6.8446	2.1690	9.1823
	DDDD	81	LEU	0.2183	0.0000	0.4367
	DDDD	82	GLU	5.8647	0.0374	10.5265
	DDDD	83	VAL	1.5404	2.6954	0.0005
10	DDDD	84	PHE	2.7805	0.6706	3.9861
10	DDDD	85	SER	6.8439	5.9428	8.6459
	DDDD	86	ASP	6.0109	2.1275	9.8943
	DODD	87	TRP	4.6976	0.2328	6.4835
	DDDD	88	LEU	0.0296	0.0530	0.0062
15	DDDD	89	LEU	0.0803	0.0002	0.1605
13	DDDD	90	LEU	0.0000	0.0000	0.0000
	DDDD	91	GLN	0.2460	0.0003	0.4426
	DDDD	92	ALA	0.0626	0.0754	0.0113
	DDDD	93	SER	4.5712	2.8665	7.9807
20	DDDD	94	ALA	8.7178	1.3188	38.3138
20	DDDD	95	GLU	7.2886	1.5976	11.8415
	DDDD	96	VAL	12.8114	4.6767	23.6578
	DDDD	97	VAL	1.4641	1.1764	1.8477
	DDDD	98	MET	13.4393	0.1457	26.7329
25	DDDD	99	GLU	7.1147	4.7251	9.0264
23	DDDD	100	GLY	5.3684	5.3684	0.0000
	DDDD	101	GLN	9.8859	0.0000	17.7946
	DDDD	102	PRO	9.5952	1.6262	20.2206
	DDDD	103	LEU	0.0075	0.0150	0.0000
30	DDDD	104	PHE	6.3221	0.0000	9.9347
30	DDDD	105	LEU	0.0690	0.0712	0.0667
	DDDD	106	ARG	2.3233	0.0001	3.6509
	DDDD	107	CYS	0.8061	1.2091	0.0000
	DDDD	108	HIS	1.1851	0.2808	1.7880
35	DDDD	109	GLY	1.2333	1.2333	0.0000
<i>J</i> J	DDDD	110	TRP	0.7404	0.3219	0.9078
	DDDD	111	ARG	7.9699	6.6124	8.7456
	DDDD	112	ASN	12.5024	3.9088	21.0960
	DDDD	113	TRP	2.0923	3.4514	1.5487
40	DDDD	114	ASP	11.6891	1.9841	21.3940
40	DDDD	115	VAL	0.8907	0.6666	1.1894
	DDDD	116	TYR	3.5406	0.0000	5.3109
	DODD	117	LYS	7.4915	0.9137	12.7537
	DDDD	118	VAL	0.0000	0.0000	0.0000
45	DDDD	119	ILE	1.5354	0.0000	3.0708
45	DOOD	120	TYR	0.0227	0.0000	0.0341
	DDDD	121	TYR	3.0000	0.0000	4.5000
	DDDD	122	LYS	3.8497	0.8215	6.2723
	DDDD	123	ASP	11.0185	7.2080	14.8291
50	DDDD	124	GLY	13.8186	13.8186	0.0000
50	DDDD	125	GLU	7.1969	0.5597	12.5066
	DODD	126	ALA	1.6231	0.9637	4.2606
	DDDD	127	LEU	5.5580	1.1317	9.9843
	DODD	128	LYS	11.0326	0.1803	19.7145
55	DDDD	129	TYR	6.0662	4.5993	6.7997
55	DDDD	130	TRP	6.9751	0.9821	9.3722

	DDDD	131	TYR	3.2844	1.1357	4.3587
	DDDD	132	GLU	10.5294	2.1545	17.2294
	DDDD	133	ASN	5.3145	5.3786	5.2503
	DDDD	134	HIS	8.2621	1.1783	12.9846
5	DDDD	135	ASN	1.2924	0.3403	2.2445
	DDDD	136	ILE	2.0846	1.3968	2.7725
	DDDD	137	SER	10.0460	7.2958	15.5465
	DDDD	138	ILE	3.5719	0.9619	6.1819
	DDDD	139	THR	16.0437	2.5113	34.0868
10	DDDD	140	ASN	6.1043	3.6342	8.5744
	DDDD	141	ALA	0.0006	0.0000	0.0028
	DDDD	142	THR	7.0414	0.4613	15.8150
	DDDD	143	VAL	7.7914	1.5021	16.1770
	DDDD	144	GLU	13.9850	4.2384	21.7824
15	DODO	145	ASP	4.1793	0.0265	8.3322
13	DDDD	146	SER	5.2665	3.1409	9.5178
	DDDD	147	GLY	3.2916	3.2916	0.0000
	DODD	148	THR	5.1835	0.0792	11.9891
	DDDD	149	TYR	0.2058	0.0000	0.3087
20	DDDD	150	TYR	3.8607	0.0000	5.7910
20	DDDD	151	CYS	0.0000	0.0000	0.0000
	DDDD	152	THR	3.9195	0.0065	9.1368
			GLY		1.0864	
	DDDD	153	LYS	1.0864	0.0302	0.0000 9.1174
25	DDDD	154	VAL	5.0786	0.0002	0.9789
25		155		0.4195	2.1135	
		156	TRP	1.3921		1.1036
	DDDD	157	GLN	5.1050	3.3675	6.4950
	DDDD	158	LEU	13.2526	0.1201	26.3851
20	DDDD	159	ASP	7.9559	2.3964	13.5153
30	DDDD	160	TYR	2.2863	2.2919	2.2835
	DDDD	161	GLU	10.7234	4.9235	15.3634
	DDDD	162	SER	1.2506	1.8759	0.0000
	DDDD	163	GLU	9.3458	0.2040	16.6593
25	DDDD	164	PRO	9.8122	1.5651	20.8083
35	DDDD	165	LEU	1.6668	0.0989	3.2347
	DDDD	166	ASN	4.0892	1.1470	7.0314
	DDDD	167	ILE	0.5690	1.1374	0.0006
	DDDD	168	THR	9.4203	0.0533	21.9098
	DDDD	169	VAL	0.5492	0.9611	0.0000
40	DDDD	170	ILE	10.5373	1.6298	19.4449
	DDDD	171	LYS	19.4334	14.2443	23.5846
	DDDD	221	NAG	12.4351	0.0000	12.4351
	DDDD	222	NAG	14.2041	0.0000	14.2041
	DDDD	242	NAG	9.7024	0.0000	9.7024
45	DDDD	243	NAG	9.7925	0.0000	9.7925
	DDDD	244	MAN	16.4248	0.0000	16.4248
	DDDD	250	NAG	15.9 65 5	0.0000	15.9655
	DDDD	274	NAG	21.7485	0.0000	21.7485
	DDDD	335	NAG	15.0635	0.0000	15.0635
50	DDDD	340	NAG	17.6569	0.0000	17.6569
	DDDD	366	NAG	14.5792	0.0000	14.5792
	DDDD	367	NAG	20.8687	0.0000	20.8687
	EEEE	4	LYS	22.3558	10.9740	31.4612
	- EEEE	5	PRO	1.1163	1.4301	0.6978
55	EEEE	6	LYS	16.9326	1.2182	29.5041
	EEEE	7	VAL	1.5370	2.6897	0.0000

	EEEE	8	SER	9.0470	1.8198	23.5014
	EEEE	9	LEU	3.7362	4.7200	2.7524
	EEEE	10	ASN	12.0492	0.9478	23.1505
_	EEEE	11	PRO	8.3799	0.5532	18.8156
5	EEEE	12	PRO	9.8266	2.0198	20.2356
	EEEE	13	TRP	1.5826	0.0955	2.1775
	EEEE	14	ASN	3.6101	0.2979	6.9223
	EEEE	15	ARG	1.6218	0.0098	2.5429
	EEEE	16	ILE	1.1456	0.0000	2.2912
10	EEEE	17	PHE	0.2563	0.0000	0.4027
	EEEE	18	LYS	10.9294	3.6992	16.7135
	EEEE	19	GLY	5.6751	5.6751	0.0000
	EEEE	20	GLU	3.4651	0.0024	6.2352
	EEEE	21	ASN	5.3587	3.9397	
15	EEEE	22	VAL	0.3206	0.4678	6.7777
	EEEE	23	THR	5.2106	0.0240	0.1243
	EEEE	24	LEU	0.2668	0.0000	12.1261
	EEEE	25	THR			0.5335
	EEEE	26	CYS	4.8755	0.0000	11.3763
20	EEEE	27	ASN	0.2422	0.3394	0.0477
20	EEEE	28		7.5792	1.5782	13.5803
	EEEE		GLY	7.7171	7.7171	0.0000
	EEEE	29	ASN	17.1451	8.1440	26.1463
		30	ASN	14.2079	9.6254	18.7903
25	EEEE	31	PHE	18.7547	8.6665	24.5194
23	EEEE	32	PHE	7.2539	7.0102 -	7.3931
	EEEE	33	GLU	17.0855	4.7908	26.9213
	EEEE	34	VAL	10.0735	3.1424	19.3149
	EEEE	35	SER	13.8902	2.0792	37.5120
20	EEEE	36	SER	6.8523	1.7904	16.9760
30	EEEE	37	THR	0.6763	1.1836	0.0000
	EEEE	38	LYS	8.3619	0.3108	14.8028
	EEEE	39	TRP	0.0083	0.0020	0.0108
	EEEE	40	PHE	3.0042	0.0000	4.7209
	EEEE	41	HIS	3.3299	0.3808	5.2960
35	EEEE	42	ASN	6.3452	7.0674	5.6231
	EEEE	43	GLY	9.6662	9.6662	0.0000
	EEEE	44	SER	12.6323	3.0497	31.7975
	EEEE	45	LEU	14.2883	6.9452	21.6315
	EEEE	46	J.JR	5.9546	3.8685	10.1268
40	EEEE	47	GĿU	19.8778	7.9851	29.3920
	EEEE	48	GLU	6.2775	2.2956	9.4630
	EEEE	49	THR	11.1492	0.0819	25.9055
	EEEE	50	ASN	3.8263	0.9910	6.6616
	EEEE	51	SER	0.9846	0.0000	2.9539
45	EEEE	52	SER	2.8049	0.0006	8.4134
	EEEE	53	LEU	2.6766	0.0083	5.3450
	EEEE	54	ASN	7.1063	3.8883	
	EEEE	55	ILE	2.1074	1.5164	10.3243
	EEEE	56	VAL	11.4388		2.6984
50	EEEE	57	ASN	8.9664	1.7734	24.3260
	EEEE	58	ALA		1.0480	16.8848
	EEEE	59	LYS	0.3426	0.4045	0.0949
	EEEE	60		13.5640	0.0175	24.4012
	EEEE		PHE	3.4104	0.0051	5.3562
55	EEEE	61	GLU	8.6064	0.1863	15.3424
<i>JJ</i>		62	ASP	4.2246	0.0962	8.3531
	EEEE	63	SER	0.1134	0.0000	0.3402

	EEEE	64	GLY	0.0266	0.0266	0.0000
	EEEE	65	GLU	4.0549	0.0880	7.2284
	EEEE	66	TYR	0.7832	0.0000	1.1748
	EEEE	67	LYS	3.2565	0.0000	5.8617
5	EEEE	68	CYS	0.0003	0.0005	0.0000
	EEEE	69	GLN	3.8454	0.0000	6.9217
	EEEE	70	HIS	2.2450	0.2224	3.5934
	EEEE	71	GLN	5.9169	3.6396	7.7387
	EEEE	72	GLN	7.4965	6.0264	8.6726
10	EEEE	73	VAL	6.4019	2.4812	11.6294
	EEEE	74	ASN	7.3226	0.8649	13.7804
	EEEE	75	GLU	9.5795	4.4019	13.7216
	EEEE	76	SER	0.7013	1.0519	0.0000
	EEEE	77	GLU	13.4227	1.1013	23.2799
15	EEEE	78	PRO	2.4705	1.5274	
15	EEEE	79	VAL	5.5768	0.7997	3.7280
	EEEE	80	TYR	3.6523	1.2328	11.9463
	EEEE	81	LEU	0.2451		4.8621
	EEEE	82	GLU	5.5763	0.0000	0.4902
20	EEEE	83	VAL		0.0256	10.0168
20	EEEE	84		1.5663	2.7355	0.0074
			PHE	2.8317	0.6685	4.0678
	EEEE	85	SER	11.1097	5.8236	21.6819
		86	ASP	6.3216	2.7103	9.9328
25	EEEE	87	TRP	9.2509	0.2339	12.8578
23	EEEE	88	LEU	0.0596	0.1001 -	0.0191
	EEEE	89	LEU	0.1011	0.0000	0.2022
	EEEE	90	LEU	0.0000	0.0000	0.0000
	EEEE	91	GLN	0.2558	0.0000	0.4604
20	EEEE	92	ALA	0.0564	0.0519	0.0745
30	EEEE	93	SER	4.5837	2.9367	7.8777
	EEEE	94	ALA	8.3906	1.2888	36. 7978
	EEEE	95	GLU	4.4296	1.5357	6.7447
	EEEE	96	VAL	4.3010	4.6742	3.8035
25	EEEE .	97	VAL	1.4250	1.0740	1.8929
35	EEEE	98	MET	13.5431	0.2108	26.8754
	EEEE	99	GLU	7.1778	4.7822	9.0943
	EEEE	100	GLY	5.0685	5.0685	0.0000
	EEEE	101	GLN	9.8626	0.0125	17.7427
	EEEE	102	PRO	9.4878	1.6105	19.9908
40	EEEE	103	LEU	0.0128	0.0246	0.0009
	EEEE	104	PHE	6.2895	0.0000	9.8835
	EEEE	105	LEU	0.0574	0.0715	0.0432
	EEEE	106	ARG	2.3284	0.0000	3.6589
	EEEE	107	CYS	0.7794	1.1691	0.0000
45	EEEE	108	HIS	1.2031	0.2846	1.8155
	EEEE	109	GLY	1.3076	1.3076	0.0000
	EEEE	110	TRP	4.3507	0.3127	5.9659
	EEEE	111	ARG	14.5626	6.7438	19.0305
	EEEE	112	ASN	12.6107	3.8715	21.3499
50	EEEE	113	TRP	7.0410	3.3592	8.5138
	EEEE	114	ASP	11.4765	1.9258	
	EEEE	115	VAL	0.8593	0.6604	21.0271
	EEEE	116	TYR	5.8929		1.1244
	EEEE	117	LYS	11.3051	0.0005	8.8392
55	EEEE	118	VAL		0.9380	19.5988
55	EEEE	119	ILE	0.0000	0.0000	0.0000
	LEEE	113	ILC	4.8820	0.0000	9.7641

	EEEE	120	TYR	0.0103	0.0000	0.0154
	EEEE	121	TYR	3.6542	0.0005	5.4811
	EEEE	122	LYS	3.7815	0.6097	6.3190
_	EEEE	123	ASP	10.9462	6.9829	14.9095
5	EEEE	124	GLY	13.7762	13.7762	0.0000
	EEEE	125	GLU	13.1766	0.5548	23.2741
	EEEE	126	ALA	14.6424	5.3245	51.9143
	EEEE	127	LEU	9.2224	5.9305	12.5143
	EEEE	128	LYS	11.5329	1.8633	19.2686
10	EEEE	129	TYR	10.3194	5.0683	12.9449
	EEEE	130	TRP	8.0715	0.9722	10.9112
	EEEE	131	TYR	11.8508	1.0518	17.2503
	EEEE	132	GLU	12.7984	2.2087	21.2701
	EEEE	133	ASN	5.2222	5.2458	5.1985
15	EEEE	134	HIS	8.275	1.2222	12.9775
	EEEE	135	ASN	1.3104	0.3410	2.2798
	EEEE .	136	ILE	2.0064	1.3737	2.6391
	EEEE	137	SER	10.1799	7.2553	16.0292
••	EEEE	138	ILE	3.5424	0.9990	6.0858
20	EEEE	139	THR	16.1230	2.4880	34.3029
	EEEE	140	ASN	6.0914	3.7069	8.4760
	EEEE	141	ALA	0.0000	0.0000	0.0000
	EEEE	142	THR	7.1532	0.3267	16.2552
~~	EEEE	143	VAL	4.0502	1.4721	7.4876
25	EEEE	144	GLU	14.1982	4.3093-	22.1094
	EEEE	145	ASP	4.2616	0.0294	8.4938
	EEEE	146	SER	5.0852	3.1109	9.0339
	EEEE	147	GLY	3.2633	3.2633	0.0000
20	EEEE	148	THR	5.3711	0.0808	12.4248
30	EEEE	149	TYR	0.2123	0.0000	0.3185
	EEEE	150	TYR	3.8241	0.0000	5.7362
	EEEE	151	CYS	0.0000	0.0000	0.0000
	EEEE	152	THR	3.8973	0.0053	9.0866
25	EEEE	153	GLY	1.0506	1.0506	0.0000
35	EEEE	154	LYS	6.3259	0.0465	11.3493
	EEEE	155	VAL	0.4347	0.0000	1.0143
	EEEE	156	TRP	10.7736	3.6761	13.6126
	EEEE	157	GLN	13.4826	3.3463	21.5916
40	EEEE	158	LEU	13.9288	. 0.1999	27.6578
40	EEEE	159	ASP	14.3643	5.1303	23.5982
	EEEE	160	TYR	3.4607	2.4956	3.9432
	EEEE	161	GLU	12.5195	4.7567	18.7297
	EEEE	162	SER	1.0778	1.6166	0.0000
45	EEEE	163	GLU	9.3641	0.1874	16.7054
45	EEEE	164	PRO	9.7812	1.5531	20.7519
	EEEE	165	LEU	1.6355	0.0916	3.1794
	EEEE	166	ASN	3.8982	1.0603	6.7362
	EEEE	167	ILE	0.5697	1.1379	0.0016
50	EEEE	168	THR	2.3606	0.0217	5.4790
50	EEEE	169	VAL	0.0074	0.0129	0.0000
	EEEE	170	ILE	2.2300	0.0089	4.4512
	EEEE	171	LYS	14.7618	13.0272	16.1495
	EEEE	221	NAG	12.9978	0.0000	12.9978
55	EEEE	222	NAG	20.1629	0.0000	20.1629
JJ	EEEE	242	NAG	8.4007	0.0000	8.4007
	EEEE	243	NAG	. 8.4488	0.0000	8.4488

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	EEEE	244	MAN '	16.3142	0.0000	16.3142
	EEEE	250	NAG	15.9751	0.0000	15.9754
	EEEE	274	NAG	18.4789	0.0000	18,4789
	EEEE	335	NAG	14.8589	0.0000	14.8589
5	EEEE	340	NAG	17.7265	0.0000	17.7265
	EEEE	366	NAG	11.7893	0.0000	11.7893
•	EEEE	367	NAG	18 5598	0.0000	18 5500

Table 10. PhFc ϵ RI α_{1-172} , Form T2, residue exposure

>>> coordinate set= pent74_11c1.pdb

	<u>segid</u>	<u>resid</u>	resname	access	access-main	access-side
	cccc	4	LYS	22.5230	10.8738	31.8424
5	CCCC	5	PRO	1.1416	1.5686	0.5722
	CCCC	6	LYS	17.1986	1.4144	29.8259
	CCCC	7	VAL	1.6270	2.8202	0.0362
	CCCC	8	SER	8.6366	1.9053	22.0990
	CCCC	9	LEU	4.4395	5.4841	3.3949
10	CCCC	10	ASN	12.0444	0.9261	23.1626
	CCCC	11	PRO	7.7510	0.4778	17.4486
	CCCC	12	PRO	10.0046	2.2549	20.3375
	CCCC	13	TRP	1.5672	0.1129	2.1488
	CCCC	14	ASN	3.3834	0.3515	6.4153
15	CCCC	15	ARG	1.7214	0.0000	2.7051
	CCCC	16	ILE	0.9799	0.0000	
	CCCC	17	PHE	0.2972	0.0000	1.9599
	CCCC	18	LYS	11.0480	3.8504	0.4670
		19	GLY	5.6439	5.6439	16.8061
20		20	GLU	3.6350		0.0000
		21	ASN	5.3939	0.0352	6.5149
		22	VAL	0.2954	4.1927	6.5951
		23	THR	5.4708	0.4493	0.0902
		24	LEU	0.4978	0.0934	12.6405
25	CCCC		THR	5.1976	0.0000 0.0006	0.9957
		26	CYS			12.1271
	CCCC		ASN	0.3073	0.3299	0.2621
		28	GLY	8.5100	1.3260	15.6940
		29	ASN	6.8597	6.8597	0.0000
30		30	ASN	17.2073	7.8659	26.5486
30		31	PHE	14.4090	9.6919	19.1261
•		\$2		18.6560	9.4593	23.9112
		33	PHE	7.3970	6.8547	7.7068
		33 34	GLU	17.4505	4.8495	27.5314
35		3 5	VAL	10.1697	3.7420	18.7399
<i>33</i>			SER	14.6634	2.2968	39.3965
		36 27	SER	7.1609	1.9487	17.5852
		37	THR	0.7165	1.2539	0.0000
		38	LYS	8.8073	0.3430	15.5788
40		39	TRP	0.0048	0.0169	0.0000
40		40	PHE	3.0629	0.0000	4.8131
		41 40	HIS	3.2953	0.2185	5.3465
		42	ASN	6.4333	7.3988	5.4678
		43	GLY	8.7787	8.7787	0.0000
45	CCCC		SER	12.5780	3.2206	31.2928
7.7	CCCC		LEU	14.3835	6.5311	22.2359
	CCCC		SER	6.0642	4.1760	9.8407
	CCCC		GLU	19.8848	8.0573	29.3468
	CCCC .		GLU	5.7325	2.1429	8.6042
50	CCCC .		THR	11.1779	0.0000	26.0818
50	CCCC		ASN	3.7291	1.0808	6.3774
	cccc	51	SER	1.1927	0.0000	3.5780

	CCCC 52	SER	2.7289	0.0000	8.1866
	CCCC 53	LEU	2.8602	0.0189	5.7014
	CCCC 54	ASN	7.0896	4.0346	10.1446
	CCCC 55	ILE	1.9722	1.4947	2.4497
5	CCCC 56	VAL	11.4466	1.8119	24.2929
	CCCC 57	ASN	9.2079	1.1203	17.2954
	CCCC 58	ALA	0.2682	0.3352	0.0000
	CCCC 59	LYS	13.5663	0.0799	24.3554
	CCCC 60	PHE	4.2653	0.0614	6.6675
10	CCCC 61	GLU	9.3104	0.1429	16.6444
	CCCC 62	ASP	4.1004	0.0929	8.1079
	CCCC 63	SER	0.1952	0.0000	0.5857
	CCCC 64	GLY	0.0000	0.0000	0.0000
	CCCC 65	GLU	3.3950	0.0904	6.0387
15	CCCC 66	TYR	1.0210	0.0004	1.5313
	CCCC 67	LYS	3.2922	0.0006	5.9255
	CCCC 68	CYS	0.0000	0.0000	0.0000
	CCCC 69	GLN	4.0273	0.0000	7.2491
	CCCC 70	HIS	2.4293	0.2618	3.8743
20	CCCC 71	GLN	10.1947	6.5416	23.8992
_•	CCCC 72	GLN	18.7079	6.7237	28.2952
	CCCC 73	VAL	5.9018	2.0768	11.0019
	CCCC 74	ASN	7.6674	1.2523	
	CCCC 75	GLU	9.5618	4.3436	14.0824
25	CCCC 76	SER	0.7453	1.1107	13.7363
23	CCCC 77	GLU	13.4902	1.2113	0.0146
	CCCC 78	PRO	3.7570		23.3134
	CCCC 79	VAL	6.27 8 6	2.4424	5.5097
	CCCC 80	TYR	4.8276	1.0035	13.3121
30	CCCC 81	LEU	0.4499	1.6806	6.4011
50	CCCC 82	GLU		0.0000	0.8998
	CCCC 83	VAL	6.0083	0.0302	10.7907
	CCCC 84	PHE	1.5038	2.6317	0.0000
	CCCC 85	SER	2.9396	0.6034	4.2746
35 ′	CCCC 86	ASP	11.0379	5.9825	21.1488
55	CCCC 87		6.6954	2.8722	10.5186
	CCCC 88	TRP	5.7551	0.2523	7.9563
	CCCC 89	LEU LEU	0.0496	0.0992	0.0000
			0.0722	0.0000	0.1444
40		LEU	0.0039	0.0006	0.0071
70	CCCC 91 CCCC 92	GLN	0.2715	0.0000	0.4886
	CCCC 92	ALA	0.1064	0.1238	0.0367
		SER	4.5560	3.0073	7.6533
	CCCC 94	ALA	8.2925	1.3979	35.8708
45	CCCC 95	GLU	5.1869	1.5220	8.1188
43	CCCC 96	VAL	5.3247	4.5540	6.3524
	CCCC 97	VAL	1.5905	0.9728	2.4141
	CCCC 98	MET	14.3166	0.0743	28.5590
	CCCC 99	GLU	7.0891	5.0739	8.7013
50	CCCC 100	GLY	5.1879	5.1879	0.0000
30	CCCC 101	GLN	9.5976	0.0133	17.2651
	CCCC 102	PRO	9.4229	1.5439	19.9284
	CCCC 103	LEU	0.0333	0.0371	0.0295
	CCCC 104	PHE	6.3516	0.0000	9.9811
55	CCCC 105	LEU	0.1059	0.0591	0.1526
55	CCCC 106	ARG	2.2520	0.0000	3.5388
	CCCC 107	CYS	0.6406	0.9609	0.0000

	CCCC 108	HIS	1.1793	0.2252	1.8153
	CCCC 109	GLY	1.3114	1.3114	0.0000
	CCCC 110	TRP	4.6295	0.3368	6.3465
	CCCC 111	ARG	13.1248	6.9961	16.6270
5	CCCC 112	ASN	12.8011	4.3120	21.2901
	CCCC 113	TRP	6.0437	3.3401	7.1251
	CCCC 114	ASP	11.9344	1.8804	21.9884
	CCCC 115	VAL	0.9151	0.7229	1.1714
	CCCC 116	TYR	5.9569	0.0000	8.9354
10	CCCC 117	LYS	11.0444	0.6651	19.3478
	CCCC 118	VAL	0.0000	0.0000	0.0000
	CCCC 119	ILE	4.4790	0.0001	8.9579
	CCCC 120	TYR	0.0043	0.0000`	0.0064
	CCCC 121	TYR	3.7210	0.0085	5.5773
15	CCCC 122	LYS	4.0141	0.9317	6.4800
	CCCC 123	ASP	10.8032	6.5278	15.0786
	CCCC 124	GLY	14.5419	14.5419	0.0000
	CCCC 125	GLU	12.8310	0.4067	22.7705
	CCCC 126	ALA	14.9558	5.5670	52.5110
20	CCCC 127	LEU	9.4777	6.3362	12.6193
	CCCC 128	LYS	11.7644	1.7577	
	CCCC 129	TYR	10.4250	4.9480	19.7697
	CCCC 130	TRP	8.2395	1.0761	13.1636
	CCCC 131	TYR	12.1293	0.8795	11.1049
25	CCCC 132	GLU	12.7495	1.9453	17.7543
	CCCC 133	ASN	5.6282	5.4710	21.3930
	CCCC 134	HIS	8.2353		5.7854
	CCCC 135	ASN	1.3610	1.4518	12.7576
	CCCC 136	ILE	2.1395	0.3583	2.3637
30	CCCC 137	SER	10.0045	1.3206	2.9584
	CCCC 138	ILE	3.5461	7.3132	15.3872
	CCCC 139	THR		0.8905	6.2017
	CCCC 140	ASN	15.6326	2.4796	33.1700
	CCCC 141	ALA	6.4183	3.6583	9.1784
35	CCCC 141	THR	0.0002	0.0000	0.0009
33	CCCC 143	VAL	7.3418	0.3932	16.6068
	CCCC 143	GLU	5.5574	1.0899	11.5140
	CCCC 145	ASP	14.2578	4.3490	22.1849
	CCCC 146	SER	4.1649	0.0654	8.2644
40	CCCC 146	GLY	5.4994	3.9946	8.5092
70	CCCC 147	THR	2.9610	2.9610	0.0000
	CCCC 148	TYR	5.8295	0.0862	13.4873
			0.2839	0.0098	0.4210
		TYR	3.8352	0.0141	5.7458
45		CYS	0.0000	0.0000	0.0000
73	CCCC 152 CCCC 153	THR	3.7535	0.0000	8.7581
		GLY	1.0847	1.0847	0.0000
		LYS	6.0253	0.0000	10.8456
		VAL	0.4796	0.0000	1.1192
50	CCCC 156	TRP	5.6483	5.3816	5.7550
50	CCCC 157	GLN	13.9764	3.1848	22.6098
	CCCC 158	LEU	9.4587	0.2983	18.6191
	CCCC 159	ASP	14.1094	4.9876	23.2312
	CCCC 160	TYR	2.5046	2.3069	2.6034
55	CCCC 161	GLU	13.4023	4.9331	20.1776
55	CCCC 162	SER	1.0596	1.5893	0.0000
	CCCC 163	GLU	9.9946	0.7061	17.4254
				•	

	CCCC 164	PRO	10.2249	1.5777	21.7546
	CCCC 165	LEU	1.6401	0.1628	3.1175
	CCCC 166	ASN	3.3684	1.0069	5.7299
	CCCC 167	ILE	0.5437	1.0633	0.0240
5	CCCC 168	THR	4.2337	0.0946	9.7525
•	CCCC 169	VAL	0.1117	0.1954	
	CCCC 170	ILE	2.4168	0.0906	0.0000 4.7430
	CCCC 171	LYS	14.4505	13.2729	
	CCCC 221	NAG	13.3692		15.3926
10	CCCC 222	NAG	19.4652	0.0000	13.3692
10	CCCC 242	NAG		0.0000	19.4652
	CCCC 242	NAG	9.4466	0.0000	9.4466
	CCCC 243	MAN	8.1868	0.0000	8.1868
	CCCC 244		18.7031	0.0000	18.7031
15	CCCC 250	NAG	16.1904	0.0000	16.1904
13	CCCC 274	NAG	21.9195	0.0000	21.9195
		NAG	15.0294	0.0000	15.0294
	CCCC 340 CCCC 366 **	NAG	17.5228	0.0000	17.5228
	0000	NAG	12.1164	0.0000	12.1164
20	CCCC 367	NAG	19.5921	0.0000	19.5921
20	AAAA 4	LYS	20.9627	10.5913	29.2599
	AAAA 5	PRO	1.1603	1.5921	0.5846
	AAAA 6	LYS	16.7967	1.3698	29.1382
	AAAA 7	VAL	1.6748	2.8323	0.1316
25	AAAA 8	SER	8.1802	1.8708	20.7991
25	AAAA 9	LEU	4.4389	5.4321	3.4456
	AAAA 10	ASN	12.2932	0.9523	23.6341
	AAAA 11	PRO	7.8292	0.4916	17.6128
	AAAA 12	PRO	9.7721	2.2628	19.7845
20	AAAA 13	TRP	1.5676	0.0823	2.1617
30	AAAA 14	ASN	3.0526	0.3315	5.7738
	AAAA 15	ARG	1.7626	0.0011	2.7691
	AAAA 16	ILE	0.9627	0.0000	1.9254
	AAAA 17	PHE	0.3249	0.0000	0.5105
	AAAA 18	LYS	10.8420	3.4841	16.7283
35	AAAA 19	GLY	5.4381	5.4381	0.0000
	AAAA 20	GLU	3.6790	0.0263	6.6011
	AAAA 21	ASN	5.3743	4.2040	6.5445
	AAAA 22	VAL	0.2940	0.4433	0.0951
40	AAAA 23	THR	5.8035	0.1030	13.4041
40	AAAA 24	LEU	0.4614	0.0000	0.9228
	AAAA 25	THR	5.1305	0.0007	11.9704
	AAAA 26	CYS	0.2915	0.3512	0.1723
	AAAA 27	ASN	6.2421	1.5400	10.9443
	AAAA 28	GLY	6.9474	6.9474	0.0000
45	AAAA 29	ASN	17.1386	8.6715	25.6057
	AAAA 30	ASN	14.4072	9.6995	19.1150
	AAAA 31	PHE	15.4860	6.5595	20.5869
	AAAA 32	PHE	3.7024	5.7813	2.5144
	AAAA 33	GLU	6.0657	4.8688	7.0232
50	AAAA 34	VAL	5.5276	3.8118	7.8153
	AAAA 35	SER	14.1613	2.3658	37.7522
	AAAA 36	SER	7.1159	1.7815	17.7848
	AAAA 37	THR	0.7225	1.2641	0.0004
	AAAA 38	LYS	8.7294	0.3364	15.4439
55	AAAA 39	TRP	0.0092	0.0322	0.0000
	AAAA 40	PHE	3.1015	0.0000	4.8738

	AAAA 41	HIS	3.4263	0.4703	5.3969
	AAAA 42	ASN	6.4271	7.3557	5.4985
	AAAA 43	GLY	8.7869	8.7869	0.0000
	AAAA 44	SER	12.6493	3.0960	31.7559
5	AAAA 45	LEU	14.5777	6.7914	
3	AAAA 46	SER	5.5814		22.3640
				3.9481	8.8482
		GLU	19.7555	7.9429	29.2055
	AAAA 48	GLU	5.9957	2.0924	9.1182
	AAAA 49	THR	11.1755	0.0000	26.0762
10	AAAA 50	ASN	3.7477	1.0911	6.4042
	AAAA 51	SER	1.1636	0.0000	3.4907
	AAAA 52	SER	2.7526	0.0004	8.2570
	AAAA 53	LEU	2.9437	0.0016	5.8859
	AAAA 54	ASN	7.0747	3.8236	10.3258
15	AAAA 55	ILE	1.9632	1.5156	2.4109
•	AAAA 56	VAL	11.4314	1.7967	24.2777
	AAAA 57	ASN	8.8194	1.1924	16.4463
	AAAA 58	ALA	0.3818	0.4773	0.0000
	AAAA 59	LYS	14.0268	0.1179	25.1539
20	AAAA 60	PHE	4.2543	0.0600	
	AAAA 61	GLU	9.3832		6.6511
	AAAA 62	ASP		0.1346	16.7820
	AAAA 63		4.0523	0.0770	8.0275
		SER	0.1601	0.0000	0.4802
25	AAAA 64	GLY	0.0003	0.0003	0.0000
23	AAAA 65	GLU	7.8567	0.0750	14.0821
	AAAA 66	TYR	1.0215	0.0000	1.5322
	AAAA 67	LYS	3.3027	0.0000	5.9449
	AAAA 68	CYS	0.0000	0.0000	0.0000
20	AAAA 69	GLN	3.9650	0.0000	7.1371
30	AAAA 70	HIS	1.3538	0.2724	2.0747
	AAAA 71	GLN	16.3949	6.5138	24.2997
	AAAA 72	GLN	18.9827	6.9646	28.5973
	AAAA 73	VAL	4.9867	2.0211	8.9408
	AAAA 74	ASN	7.4791	1.0651	13.8931
35	AAAA 75	GLU	9.6144	4.2579	13.8996
	AAAA 76	SER	0.6674	0.9903	0.0214
	AAAA 77	GLU	15.9242	1.2854	27.6353
	AAAA 78	PRO	8.1677	4.8944	12.5320
•	AAAA 79	VAL	6.4525	1.5909	12.9345
40	AAAA 80	TYR	7.2923	1.8827	9.9971
	AAAA 81	LEU	0.4642	0.0000	0.9283
	AAAA 82	GLU	6.0060	0.0321	10.7852
	AAAA 83	VAL	1.5422	2.6988	0.0000
	AAAA 84	PHE	2.9572	0.6545	4.2730
45	AAAA 85	SER	10.8486	6.1560	20.2338
	AAAA 86	ASP	6.1844	2.2433	
	AAAA 87	TRP	9.3655		10.1256
	AAAA 88	LEU		0.2163	13.0252
	AAAA 89	LEU	0.0504	0.1008	0.0000
50	AAAA 90		0.1469	0.0000	0.2937
50		LEU	0.0016	0.0007	0.0025
		GLN	0.2732	0.0066	0.4865
	AAAA 92	ALA	0.0432	0.0426	0.0458
	AAAA 93	SER	4.4502	2.9733	7.4040
55	AAAA 94	ALA	8.7362	1.3963	38.0959
55	AAAA 95	GLU	7.1768	1.5655	11.6658
	AAAA 96	VAL	13.5692	4.6624	25.4450

	AAAA 97	VAL	1.5462	0.9380	2.3571
	AAAA .98	MET	14.3960	0.0702	28.7219
	AAAA 99	GLU	7.3826	4.6030	9.6063
_	AAAA 100	GLY	4.9867	4.9867	0.0000
5	AAAA 101	GLN	9.6618	0.0164	17.3782
	AAAA 102	PRO	9.4982	1.5257	20.1283
	AAAA 103	LEU	0.0170	0.0095	0.0245
	AAAA 104	PHE	6.3600	0.0000	9.9943
	AAAA 105	LEU	0.0964	0.0678	0.1250
10	AAAA 106	ARG	2.2271	0.0002	3.4997
	AAAA 107	CYS	0.6410	0.9615	0.0000
	AAAA 108	HIS	1.1779	0.2061	1.8257
	AAAA 109	GLY	1.2835	1.2835	0.0000
15	AAAA 110	TRP	4.3852	0.3446	6.0014
15	AAAA 111	ARG	14.5965	6.9788	18.9495
	AAAA 112 AAAA 113	ASN	13.1375	4.4344	21.8406
	AAAA 113 · AAAA 114	TRP	7.1680	3.4865	8.6407
	AAAA 115	ASP	11.7831	1.8946	21.6716
20		VAL	0.9352	0.7629	1.1650
20	AAAA 116 AAAA 117	TYR	5.3542	0.0000	8.0313
	AAAA 117	LYS VAL	7.2506	0.7461	12.4542
	AAAA 119	ILE	0.0000	0.0000	0.0000
	AAAA 120	TYR	1.6994 0.0315	0.0000 0.0007	3.3988
25	AAAA 121	TYR	2.9781	0.0007	0.0469
~3	AAAA 122	LYS	3.9855	0.7635	4.4667
	AAAA 123	ASP	10.6844	6.3101	6.5630
	AAAA 124	GLY	14.6459	14.6459	15.0587
	AAAA 125	GLU	7.8188	0.3898	0.0000 13.7619
30	AAAA 126	ALA	2.0714	1.0926	5.9866
	AAAA 127	LEU	5.8795	1.4447	10.3142
	AAAA 128	LYS	11.0255	0.1820	19.7002
	AAAA 129	TYR	5.6220	4.2110	6.3275
	AAAA 130	TRP	6.9643	1.0858	9.3157
35	AAAA 131	TYR	2.7608	0.9482	3.6671
	AAAA 132	GLU	9.8508	1.9760	16.1507
	AAAA 133	ASN	5.7009	5.5383	5.8635
	AAAA 134	HIS	8.0039	1.5080	12.3344
	AAAA 135	ASN	1.3397	0.3105	2.3689
40	AAAA 136	ILE	2.1821	1.3384	3.0258
	AAAA 137	SER	9.9955	7.3477	15.2912
	AAAA 138	ILE	3.4842	0.8752	6.0933
	AAAA 139	THR	15.7464	2.4744	33.4424
	AAAA 140	ASN	6.4552	3.7317	9.1786
45	AAAA 141	ALA	0.0000	0.0000	0.0000
	AAAA 142	THR	7.4724	0.4042	16.8967
	AAAA 143	VAL	7.7469	1.0561	16.6680
	AAAA 144	GLU	14.1113	4.3219	21.9429
50	AAAA 145	ASP	4.3240	0.0500	8.5980
50	AAAA 146	SER	5.4853	4.0599	8.3361
	AAAA 147	GLY	2.8492	2.8492	0.0000
	AAAA 148	THR	5.7830	0.0884	13.3757
	AAAA 149	TYR	0.2720	0.0018	0.4071
66	AAAA 150	TYR	3.9253	0.0098	5.8831
55	AAAA 151	CYS	0.0000	0.0000	0.0000
	AAAA 152	THR	3.7350	0.0000	8.7151

	AAAA	153	GLY	1.0268	1.0268	0.0000
	AAAA	154	LYS	4.9160	0.0084	8.8421
	AAAA	155	VAL	0.4691	0.0000	1.0946
	AAAA	156	TRP	11.7056	5.3116	14.2632
5	AAAA	157	GLN	9.2515	3.3242	13.9933
	AAAA	158	LEU	13.8847	0.2727	27.4967
	AAAA	159	ASP	9.2336	3.2139	15.2533
	AAAA	160	TYR	3.5492	2.3626	4.1425
	AAAA	161	GLU	11.2704	5.0419	16.2531
10	AAAA	162	SER	1.1125	1.6687	0.0000
	AAAA	163	GLU	9.7709	0.4328	17.2413
	AAAA	164	PRO	10.3588	1.5740	22.0717
	AAAA	165	LEU	1.6439	0.1655	3.1223
1.5	AAAA	166	ASN	4.0686	1.1039	7.0332
15	AAAA	167	ILE	0.5158	1.0240	0.0075
	AAAA	168	THR	10.0323	0.1297	23.2358
	AAAA	169	VAL	0.5330	0.8959	0.0491
	AAAA	170	ILE	10.6523	1.5082	19.7963
20	AAAA	171	LYS	20.1585	15.5532	23.8428
20	AAAA	221	NAG	13 2449	0.0000	13.2449
	AAAA AAAA	222 242	NAG	19.9892	-0.0000	19.9892
	AAAA	242 243	NAG	9.9407	0.0000	9.9407
	AAAA	243 244	NAG	9.4600	0.0000	9.4600
25	AAAA	250	MAN NAG	18.6631	0.0000	18.6631
23	AAAA	274	NAG	16.3080 21.8749	0.0000	16.3080
	AAAA	335	NAG	15.0157	0.0000 0.0000	21.8749
	AAAA	340	NAG	17.2280	0.0000	15.0157
	AAAA	366	NAG	14.4545	0.0000	17.2280
30	AAAA	367	NAG	20.9042	0.0000	14.4545 20.9042
	BBBB	4	LYS	22.4434	10.6722	31.8604
	BBBB	5	PRO	1.1609	1.5819	0.5996
	BBBB	6	LYS	16.5842	1.4102	28.7235
	BBBB	7	VAL	1.6862	2.8240	0.1692
35	BBBB	8	SER	8.2982	1.8668	21.1609
	BBBB	9	LEU	4.4129	5.4051	3.4206
	BBBB	10	ASN	11.9525	0.9175	22.9875
	BBBB	11	PRO	7.8250	0.4752	17.6248
	BBBB	12	PRO	10.1980	2.1957	20.8677
40	BBBB	13	TRP	1.5849	0.0977	2.1798
	BBBB	14	ASN	3.3380	0.3318	6.3443
	BBBB	15	ARG	1.7418	0.0000	2.7372
	BBBB	16	ILE	0.9354	0.0001	1.8707
	BBBB	17	PHE	0.3221	0.0000	0.5062
45	BBBB	18	LYS	11.1312	3.8205	16.9798
	BBBB	19	GLY	5.3141	5.3141	0.0000
	BBBB	20	GLU	3.5506	0.0401	6.3590
	BBBB	21	ASN	5.3304	4.1079	6.5530
50	BBBB	22	VAL	0.2845	0.4466	0.0683
50	BBBB	23	THR	5.5150	0.0841	12.7561
	BBBB	24	LEU	0.4740	0.0000	0.9480
	BBBB	25	THR	5.1331	0.0000	11.9772
	8888	26	CYS	0.2892	0.3174	0.2327
55	BBBB	27	ASN	6.4305	1.5210	11.3399
J	BBBB	28	GLY	7.2421	7.2421	0.0000
	BBBB	29	ASN	17.3886	8.6086	26.1686

		•			
	BBBB 30	ASN	14.2633	10.0072	18.5194
	BBBB 31	PHE	18.8528	9.5505	24.1684
	BBBB 32	PHE	6.5037	6.5617	6.4706
	BBBB 33	GLU	12.9342	4.8992	19.3623
5	BBBB 34	VAL	8.3666	3.8085	14.4440
_	BBBB 35	SER	14.2536	2.2580	38.2448
	BBBB 36	SER	7.1333	1.8956	17.6087
	BBBB 37	THR	0.7187	1.2577	
	BBBB 38	LYS	8.8478	0.3137	0.0000
10	BBBB 39	TRP	0.0155	0.0288	15.6751
10	BBB8 40	PHE	3.1021	0.0000	0.0102
	BBBB 41	HIS	3.3964		4.8747
	BBBB 42	ASN	4.3570	0.4181	5.3819
	BBBB 43	GLY		5.3484	3.3656
15	BBBB 44	SER	8.6389	8.6389	0.0000
15	BBBB 45	LEU	12.5229	3.2589	31.0508
	BBBB 46		14.4289	6.6263	22.2316
	BBBB 47	SER	6.1946	4.5349	9.5141
		GLU	19.7813	8.0788	29.1432
20	BBBB 48	GLU	5.7938	2.2706	8.6124
20	BBBB 49	THR	11.0771	0.0000	25.8466
	BBBB 50	ASN	3.6499	1.0731	6.2267
	BBBB 51	SER	1.1954	0.0005	3.5851
	BBBB 52	SER	2.7282	0.0002	8.1843
25	BBBB 53	LEU	2.6801	0.0033	5.3570
25	BBBB 54	ASN	7.0535	4.0402	10.0668
	BBBB 55	ILE	1.9823	1.5180	2.4466
	BBBB 56	VAL	11.5628	1.8317	24.5377
	BBBB 57	ASN	8.8810	1.1220	16.6400
20	BBBB 58	ALA	0.3193	0.3991	0.0000
30	BBBB 59	LYS	13.7310	0.1005	24.6353
	BBBB 60	PHE	4.2410	0.1526	6.5772
	BBBB 61	GLU	9.1821	0.1249	16.4278
	BBBB 62	ASP	4.1444	0.0742	8.2145
~~	BBBB 63	SER	0.1404	0.0003	0.4207
35	BBBB 64	GLY	0.0115	0.0115	0.0000
	BBBB 65	GLU	7.8724	0.0613	14.1212
	BBBB 66	TYR	1.0150	0.0106	1.5171
	BBBB 67	LYS	3.3196	0.0000	5.9752
40	BBBB 68	CYS	0.0000	0.0000	0.0000
40	BBBB 69	GLN	4.0029	0.0000	7.2052
	BBBB 70	HIS	1.6317	0.2424	2.5580
	BBBB 71	GLN	13.5234	6.2391	19.3508
	BBBB 72	GLN	13.7415	5.5049	20.3307
	BBBB 73	VAL	3.0796	1.9941	4.5269
45	BBBB 74	ASN	7.4362	0.9858	13.8867
	BBBB 75	GLU	9.6630	4.3598	13.9056
	BBBB 76	SER	0.6085	0.9051	0.0153
	8888 77	GLU	15.8267	1.2423	27.4942
	BBBB 78	PRO	8.2618	4.8501	12.8107
50	BBBB 79	VAL	6.6038	1.6215	13.2470
	BBBB 80	TYR	7.2918	1.9227	9.9763
	BBBB 81	LEU	0.4359	0.0011	0.8708
	BBBB 82	GLU	5.5353	0.0340	9.9364
	BBBB 83	VAL	1.5227	2.6648	0.0000
55	BBBB 84	PHE	2.9287	0.6127	4.2522
	BBBB 85	SER	11.1963	6.1246	21.3396

	BBBB 86	ASP	6.4970	2.8341	10.1599
	BBBB 87	TRP	9.3025	0.2173	12.9366
	BBBB 88	LEU	0.0466	0.0933	0.0000
	BBBB 89	LEU	0.1325	0.0000	0.2650
5	BBBB 90	LEU	0.0000	0.0000	0.0000
	BBBB 91	GLN	0.2/15	0.0001	0.4887
	BBBB 92	ALA	0.1140	0.1208	0.0870
	BBBB 93	SER	4.3701	3.0355	7.0392
	BBBB 94	ALA	8.8274	1.4714	38.2514
10	BBBB 95	GLU	7.1968	1.4526	11.7922
	BBBB 96	VAL	13.4385	4.5929	25.2325
	BBBB 97	VAL	1.5907	0.9613	2.4301
	BBBB 98	MET	14.3698	0.0738	28.6658
	BBBB 99	GLU	7.3281	4.9392	9.2392
15	BBBB 100	GLY	5.257	5.2577	0.0000
	BBBB 101	GLN	9.4091	0.0245	16.9168
	BBBB 102	PRO	9.6291	1.5760	20.3666
	BBBB 103	LEU	0.0129	0.0053	0.0206
	BBBB 104	PHE	6.1594	0.0000	9.6790
20	BBBB 105	LEU	0.0613	0.0533	0.0693
	BBBB 106	ARG	2.2836	0.0000	3.5885
	BBBB 107	CYS	0.6725	1.0088	0.0000
	BBBB 108	HIS	1.1253	0.2267	1.7244
	BBBB 109	GLY	1.2775	1.2775	0.0000
25	BBBB 110	TRP	4.4509	0.3060	6.1089
	BBBB 111	ARG	14.4604	6.9977	18.7248
	BBBB 112	ASN	13.1855	4.3879	21.9831
	BBBB 113	TRP	7.1019	3.5603	8.5186
	BBBB 114	ASP	11.9934	2.2124	21.7745
30	BBBB 115	VAL	0.9738	0.8493	1.1398
	BBBB 116	TYR	5.9699	0.0003	8.9548
	BBBB 117	LYS	11.3675	0.6641	19.9301
	BBBB 118	VAL	0.0000	0.0000	0.0000
	. BBBB 119	ILE	4.4231	0.0000	8.8463
35	BBBB 120	TYR	0.0060	0.0000	0.0090
	BBBB 121	TYR	3.5477	0.0003	5.3215
	BBBB 122	LYS	3.9640	0.7211	6.5584
	BBBB 123	ASP	10.6309	6.1402	15.1215
	BBBB 124	GLY	14.3673	14.3673	0.0000
40	BBBB 125	GLU	13.1648	0.4047	23.3729
	BBBB 126	ALA	14.7406	5.6401	51.1429
	BBBB 127	LEU	9.0669	6.2840	11.8498
	BBBB 128	LYS	11.7318	1.7962	19.6802
	BBBB 129	TYR	10.3977	5.0068	13.0932
45	BBBB 130	TRP	8.0404	1.1151	10.8105
	BBBB 131	TYR	12.1527	0.8656	17.7962
	BBBB 132	GLU	12.6929	2.0269	21.2256
	BBBB 133	ASN	5.5740	5.4313	5.7167
	BBBB 134	HIS	8.2722	1.4837	12.7979
50	BBBB 135	ASN	1.3495	0.3379	2.3611
	BBBB 136	ILE	2.1772	1.2842	3.0701
	BBBB 137	SER	10.0581	7.4531	15.2681
	BBBB 138	ILE	3.4589	0.9040	6.0137
	BBBB 139	THR	15.5520	2.5023	32.9516
55	BBBB 140	ASN	6.4140	3.6881	9.1399
	BBBB 141	ALA	0.0003	0.0003	0.0000

	BB8B 142	THR	6.5774	0.3047	14.9409
	BBBB 143	VAL	7.8299	1.0449	16.8764
	BBBB 144	GLU	14.1982	4.2567	22.1514
	BBBB 145	ASP	4.3806	0.0466	8.7146
5	BBBB 146	SER	5.5841	4.1811	8.3902
	BBBB 147	GLY	2.9485	2.9485	0.0000
	BBBB 148	THR	5.5009	0.1035	12.6974
	BBBB 149	TYR	0.2416	0.0180	0.3534
	BBBB 150	TYR	3.8781	0.0000	5.8171
10	BBBB 151	CYS	0.0000	0.0000	0.0000
	BBBB 152	THR	3.8579	0.0000	9.0018
	BBBB 153	GLY	1.0286	1.0286	0.0000
	BBBB 154	LYS	6.0883	0.0037	10.956 1
	BBBB 155	VAL	0.4604	0.0000	1.0742
15	BBBB 156	TRP	11.6843	J.2412	14.2615
	BBBB 157	GLN	14.2169	3.2783	22.9678
	BBBB 158	LEU	13.8111	0.3293	27.2930
	BBBB 159	ASP	14.3170	4.9359	23.6980
00	BBBB 160	TYR	3.5010	2.3021	4.1004
20	BBBB 161	GLU	13.3785	5.0194	20.0658
	BBBB 162	SER	1.1216	1.6824	0.0000
	BBBB 163	GLU	9.8626	0.5373	17.3229
	BBBB 164	PRO	10.0802	1.5190	21.4953
25	BBBB 165	LEU	1.6748	0.1571	3.1924
25	BBBB 166	ASN	4.0864	1.0418	7.1311
	BBBB 167	ILE	0.5430	1.0598	0.0262
	BBBB 168 BBBB 169	THR	9.9575	0.1056	23.0934
	BBBB 169 BBBB 170	VAL	0.5482	0.9594	0.0000
30	BBBB 171	ILE LYS	10.7170	1.5437	19.8904
30	BBBB 221	NAG	20.1725 13.1802	15.3137 0.0000	24.0596
	BBBB 222	NAG	20.4108	0.0000	13.1802
	BBBB 242	NAG	7.5051	0.0000	20.4108 7.5051
	BBBB 243	NAG	7.8194	0.0000	7.8194
35	BBBB 244	MAN	18.6420	0.0000	18.6420
, ,	BBBB 250	NAG	16.2628	0.0000	16.2628
	BBBB 274	NAG	21.8856	0.0000	21.8856
	BBBB 335	NAG	14.8369	0.0000	14.8369
	BBBB 340	NAG	17.4016	0.0000	17.4016
40	BBBB 366	NAG	14.6038	0.0000	14.6038
	BBBB 367	NAG	21.0874	0.0000	21.0874
	DDDD 4	LYS	22,1244	10.4757	31.4434
	DDDD 5	PRO	1.1536	1.5927	0.5680
	DDDD 6	LYS	17.0471	1.3682	29.5902
45	DDDD 7	VAL	1.6664	2.8596	0.0755
	DDDD 8	SER	8.3148	1.8918	21.1607
	DDDD 9	LEU	4.3290	5.2653	3.3927
	DDDD 10	ASN	12.0081	0.9613	23.0549
	DDDD 11	PRO	8.1330	0.4813	18.3353
50	DDDD 12	PRO	10.2920	2.3028	20.9442
	DDDD 13	TRP	1.5549	0.0701	2.1488
	DDDD 14	ASN	3.1974	0.3117	6.0832
	DDDD 15	ARG	1.7368	0.0000	2.7293
	DDDD 16	ILE	0.9559	0.0003	1.9114
55	DDDD 17	PHE	0.3209	0.0000	0.5043
	DDDD 18	LYS	10.9142	3.4868	16.8562

	DDDD 19	GLY	5.8859	5.8859	0.0000
	DDDD 20	GLU	3.5184	0.0001	6.3330
	DDDD 21	ASN	5.3913	4.1153	6.6672
_	DDDD 22	VAL	0.2777	0.4369	0.0655
5	DDDD 23	THR	5.8162	0.1076	13.4277
	DDDD 24	LEU	0.4623	0.0006	0.9240
	DDDD 25	THR	5.1763	0.0000	12.0779
	DDDD 26	CYS	0.2817	0.3216	0.2020
10	DDDD 27	ASN	8.2286	1.5680	14.8891
10	DDDD 28	GLY	7.4834	7.4834	0.0000
	DDDD 29	ASN	17.4431	8.5265	26.3597
	DDDD 30	ASN	14.3278	10.0224	18.6333
	DDDD 31	PHE	18.8219	8.9687	24.4524
15	DDDD 32 DDDD 33	PHE	7.0915	6.7608	7.2806
13	DDDD 33 DDDD 34	GLU VAL	17.4529	5.1261	27.3143
	DDDD 35	SER	10.0069	3.7179	18.3922
	DDDD 36	SER	14.6436	2.2454	39.4399
	DDDD 37	THR	7.1471 0.7333	1.9242 1.2833	17.5931
20	DDDD 38	LYS	8.80 5 8		0.0000
20	DDDD 39	TRP	0.0167	0.3191 0.0569	15.5951
	DDDD 40	PHE	3.0699	0.0000	0.0007
	DDDD 41	HIS	3.3244	0.1639	4.8241
	DDDD 42	ASN	6.2564	7.1984	5.4315 5.3143
25	DDDD 43	GLY	8.8245	8.8245	0.0000
	DDDD 44	SER	12.8423	3.1760	32.1749
	DDDD 45	LEU	14.8050	7.3234	22.2866
	DDDD 46	SER	6.2461	4.5119	9.7144
	DDDD 47	GLU	19.8403	7.8973	29.3948
30	DDDD 48	GLU	5.7613	2.1656	8.6379
	DDDD 49	THR	10.9341	0.0000	25.5128
	DDDD 50	ASN	3.7321	1.0782	6.3860
	DDDD 51	SER	1.1905	0.0000	3.5714
	DDDD 52	SER	2.7666	0.0003	8.2993
35	DDDD 53	LEU	2.7642	0.0050	5.5234
	DDDD 54	ASN	7.1762	4.1170	10.2353
	DDDD 55	ILE	1.9872	1.4615	2.5130
	DDDD 56	VAL	11.4848	1.8199	24.3713
40	DDDD 57	ASN	9.2650	1.2272	17.3029
40	DDDD 58	ALA	0.3308	0.4134	0.0000
	DDDD 59	LYS	13.7555	0.1261	24.6591
	DDDD 60	PHE	4.2948	0.3462	6.5511
	DDDD 61	GLU	9.1485	0.1440	16.3520
45	DDDD 62	ASP	4.0350	0.0620	8.0080
43	DDDD 63	SER	0.1959	0.0000	0.5877
	DDDD 64 DDDD 65	GLY	0.0065	0.0065	0.0000
	DDDD 65 DDDD 66	GLU	7.8394	0.0396	14.0791
	DDDD 67	TYR	1.0148	0.0000	1.5222
50	DDDD 68	LYS CYS	3.3208	0.0000	5.9774
50	DDDD 69		0.0002	0.0000	0.0005
	DDDD 70	GLN HIS	3.9726	0.0000	7.1507
	DDDD 71	GLN	2.6810 16.6353	0.2742	4.2855
	DDDD 72	GLN	16.6353 18.9785	6.3493 6.0612	24.8641
55	DDDD 73	VAL	5.8822	6.9612	28.5924
	DDDD 74	ASN	7.4325	1.9838 0.9456	11.0801
		, .514	(.7020	ń.2420	13.9195

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	DDDD 75	GLU	9.6342	4.3175	13.8875
	DDDD 76	SER	0.6597	0.9801	0.0188
	DDDD 77	GLU	15.8994	1.2593	27.6115
	DDDD 78	PRO	8.2500	4.9080	12.7060
5	DDDD 79	VAL	6.5718	1.5859	13.2197
	DDDD 80	TYR	7.3618	1.8414	10.1220
	DDDD 81	LEU	0.3727	0.0000	0.7455
	DDDD 82	GLU	5.7273	0.0000	10.3091
	DDDD 83	VAL	1.6083	2.8146	0.0000
10	DDDD 84	PHE	2.9246	0.6110	4.2466
	DDDD 85	SER	11.0966	6.0084	21.2730
	DDDD 86	ASP	6.2089	2.2133	10.2046
	DDDD 87	TRP	6.4962	0.2557	8.9923
	DDDD 88	LEU	0.0479	0.0958	0.0000
15	DDDD 89	LEU	0.1157	0.0000	0.2313
	DDDD 90	LEU	0.0002	0.0000	0.0004
	DDDD 91	GLN	0.2632	0.0000	0.4737
	DDDD 92	ALA	0.0436	0.0427	0.0472
	DDDD 93	SER	4.5089	2.9688	7.5891
20	DDDD 94	ALA	8.3925	1.3517	36.5557
	DDDD 95	GLU	7.1932	1.4693	11.7724
	DDDD 96	VAL	13.5421	4.7333	25.2870
	DDDD 97	VAL	1.5725	0.9243	2.4367
	DDDD 98	MET	14.2776	0.0883	28.4668
25	DDDD 99	GLU	7.6854	4.8779	9.9313
	DDDD 100	GLY	4.9621	4.9621	0.0000
	DDDD 101	GLN	9.7282	0.0319	17.4852
	DDDD 102	PRO	9.4269	1.5462	19.9345
	DDDD 103	LEU	0.0306	0.0330	0.0282
30	DDDD 104	PHE	6.2490	0.0000	9.8199
	DDDD 105	LEU	0.0962	0.0653	0.1272
	DDDD 106	ARG	2.2407	0.0007	3.5207
	DDDD 107	CYS	0.6463	0.9694	0.0000
0.5	DDDD 108	HIS	1.1583	0.2394	1.7709
35	DDDD 109	GLY	1.3558	1.3558	0.0000
	DDDD 110	TRP	4.6167	0.3206	6.3351
	DDDD 111	ARG	13.1658	6.9018	16.7453
	DDDD 112	ASN	12.9428	4.3861	21.4995
40	DDDD 113	TRP	6.0476	2.8196	7.3388
40	DDDD 114	ASP	11.3414	1.8363	20.8466
	DDDD 115	VAL	0.8809	0.7036	1.1174
	DDDD 116	TYR	5.3412	0.0000	8.0118
	DDDD 117	LYS	8.0269	0.7095	13.8809
45	DDDD 118 DDDD 119	VAL	0.0001	0.0000	0.0002
43		ILE	1.6342	0.0000	3.2684
	DDDD 120 DDDD 121	TYR	0.0131	0.0000	0.0197
	DDDD 121	TYR LYS	2.9992	0.0083	4.4947
	DDDD 123		4.0023	0.8041	6.5609
50	DDDD 123	ASP GLY	10.7259	6.1708	15.2810
50	DDDD 125	GLU	14.3365 7.3185	14.3365	0.0000
	DDDD 126	ALA	7.3185 2.1423	0.3720	12.8756
	DDDD 127	LEU	5.9 56 9	1.1064	6.2860
	DDDD 128	LYS	11.1254	1.4445 0.2785	10.4694
55	DDDD 129	TYR	5.7025	4.2384	19.8028 6.4346
	DDDD 130	TRP	6.8913	1.0864	9.2132
			5.5510	1.0004	3.2132

	DDDD 131	TYR	4.0982	0.8881	5.7033
	DDDD . 132	GLU	11.0810	2.0497	18.3061
	DDDD 133	ASN	5.7438	5.5427	5.9449
	DDDD 134	HIS	8.0681	1.4827	12.4583
5	DDDD 135	ASN	1.3522	0.3616	2.3429
	DDDD 136	ILE	2.1277	1.2709	2.9846
	DDDD 137	SER	10.0928	7.5360	15.2065
	DDDD 138	ILE	3.4325	0.8858	5.9792
	DDDD 139	THR	15.7856	2.5286	33.4616
10	DDDD 140	ASN	6.3849	3.6475	9.1223
	DDDD 141	ALA	0.0000	0.0000	0.0000
	DDDD 142	THR	7.3411	0.2496	16.7963
	DDDD 143	VAL	7.7635	1.1808	16.5403
	DDDD 144	GLU	13.9706	4.2430	21.7527
15	DDDD 145	ASP	4.2654	0.0465	8.4843
	DDDD 146	SER	5.4380	3.9844	8.3451
	DDDD 147	GLY	2.9908	2.9908	0.0000
	DDDD 148	THR	5.6821	0.0926	13.1348
00	DDDD 149	TYR	0.2615	0.0000	0.3922
20	DDDD 150	TYR	3.8602	0.0001	5.7903
	DDDD 151	CYS	0.0000	0.0000	0.0000
	DDDD 152	THR	3.8063	0.0000	8.8814
	DDDD 153	GLY	1.1071	1.1071	0.0000
05	DDDD 154	LYS	5.9720	0.0003	10.7494
25	DDDD 155	VAL	0.4744	0.0002	1.1066
	DDDD 156	TRP	3.1754	2.8159	3.3193
	DDDD 157	GLN	10.0034	3.2877	15.3759
	DDDD 158	LEU	14.1226	0.2738	27.9715
30	DDDD 159	ASP	7.9805	2.3321	13.6289
30	DDDD 160 DDDD 161	TYR	3.5343	2.4074	4.0978
	DDDD 161 DDDD 162	GLU	12.6759	4.6202	19.1204
	DDDD 162 DDDD 163	SER	1.1111	1.6667	0.0000
	DDDD 163	GLU PRO	9.9628	0.6047	17.4493
35	DDDD 165	LEU	10.2553	1.5732	21.8314
33	DDDD 166	ASN	1.6609	0.1704	3.1515
	DDDD 167	ILE	4.3037 0.5355	1.0892	7.5182
	DDDD 168	THR	9.9863	1.0632 0.0926	0.0079
	DDDD 169	VAI	0.5843	0.0926	23.1779
40	DDDD 170	ILE.	10.6158	1.4450	0.0466
,,	DDDD 171	LYS	20.3127	15.3369	19.7865
	DDDD 221	NAG	13.3953	0.0000	24.2933 13.3953
	DDDD 222	NAG	19.9723	0.0000	19.9723
	DDDD 242	NAG	9.9403	0.0000	9.9493
45	DDDD 243	NAG	9.3637	0.0000	9.3637
	DDDD 244	MAN	18.7429	0.0000	18.7429
	DDDD 250	NAG	16.0945	0.0000	16.0945
	DDDD 274	NAG	21.9996	0.0000	21.9996
	DDDD 335	NAG	15.1906	0.0000	15.1906
50	DDDD 340	NAG	17.8940	0.0000	17.8940
	DDDD 366	NAG	14.6791	0.0000	14.6791
	DDDD 367	NAG	20.8557	0.0000	20.8557
	EEEE 4	LYS	22.5960	10.2165	32.4995
	EEEE 5	PRO	1.1597	1.6130	0.5553
55	EEEE 6	LYS	16.8781	1.3580	29.2941
	EEEE 7	VAL	1.6131	2.7766	0.0619
					2.2010

	EEEE 8	SER	8.2297	1.9067	20.8757
	EEEE . 9	LEU	4.4542	5.4841	3.4242
	EEEE 10	ASN	11.9578	0.9345	22.9812
_	EEEE 11	PRO	8.0892	0.4787	18.2367
5	EEEE 12	PRO	10.2667	2.2261	20.9875
	EEEE 13	TRP	1.5846	0.0803	2.1863
	EEEE 14	ASN	3.3863	0.3258	6.4468
	EEEE 15	ARG	1.7357	0.0000	2.7275
	EEEE 16	ILE	0.9829	0.0000	1.9657
10	EEEE 17	PHE	0.3246	0.0002	0.5100
	EEEE 18	LYS	10.8388	3.5327	16.6837
	EEEE 19	GLY	5.3803	5.3803	0.0000
	EEEE 20	GLU	3.5458	0.0335	6.3557
15	EEEE 21	ASN	5.3181	4.0487	6.5875
15	EEEE 22	VAL	0.2825	0.4415	0.0706
	EEEE 23	THR	5.3581	0.0670	12.4128
	EEEE 24	LEU	0.4756	0.0000	0.9513
	EEEE 25	THR	5.2190	0.0000	12.1778
20	EEEE 26	CYS	0.3475	0.4090	0.2246
20	EEEE 27 EEEE 28	ASN	8.6206	1.5643	15.6770
	EEEE 28 EEEE 29	GLY	7.3744	7.3744	0.0000
	EEEE 30	ASN	16.8741	8.5078	25.2404
	EEEE 31	ASN	14.4860	9.6381	19.3339
25	EEEE 32	PHE PHE	18.9288	9.2491	24.4601
23	EEEE 33	GLU	7.2780	6.7628	7.5723
	EEEE 34	VAL	17.3 77 6 9.8146	4.9213	27.3427
	EEEE 35	SER	14.4525	3.7193 2.24 3 8	17.9417
	EEEE 36	SER	7.1292	1.8233	38.8698
30	EEEE 37	THR	0.7268	1.2719	17.7410
	EEEE 38	LYS	8.8146	0.3416	0.0000 15.5930
	EEEE 39	TRP	0.0112	0.0389	0.0002
	EEEE 40	PHE	3.0771	0.0000	4.8354
	EEEE 41	HIS	3.3339	0.3893	5.2969
35	EEEE 42	ASN	6.3403	7.2548	5.4259
	EEEE 43	GLY	8.8849	8.8849	0.0000
	EEEE 44	SER	12.3851	3.1501	30.8551
	EEEE 45	LEU	14.5997	6.7706	22.4287
	EEEE 46	SER	6.2344	4.5208	9.6615
40	EEEE 47	GLU	19.8124	8.1501	29.1422
	EEEE 48	GLU	5.5829	2.2603	8.2411
	EEEE 49	THR	11.1823	0.0000	26.0920
	EEEE 50	ASN	3.7514	1.0379	6.4648
	EEEE 51	SER	1.1628	0.0001	3.5482
45	EEEE 52	SER	2.6847	0.0000	8.0542
	EEEE 53	LEU	2.8988	0.0160	5.7815
	EEEE 54	ASN	7.0295	3.8406	10.2183
	EEEE 55	ILE	1.9774	1.5267	2.4282
50	EEEE 56	VAL	11.4385	1.7455	24.3625
50	EEEE 57	ASN	8.9737	1.1309	16.8164
	EEEE 58	ALA	0.3534	0.4418	0.0000
	EEEE 59	LYS	14.0513	0.0995	25.2128
	EEEE 60	PHE	3.9435	0.0489	6.1690
55	EEEE 61	GLU	9.2441	0.1331	16.5329
55	EEEE 62	ASP	4.0153	0.0793	7.9514
	EEEE 63	SER	. 0.1893	0.0000	0.5678

	EEEE 64	GLY	0.0000	0.0000	0.0000
	EEEE . 65	GLU	2.9838	0.0460	0.0000 5.3340
	EEEE 66	TYR	1.0048	0.0006	1.5069
	EEEE 67	LYS	3.2772	0.0001	5.8989
5	EEEE 68	CYS	0.0000	0.0000	0.0000
	EEEE 69	GLN	3.9654	0.0000	7.1378
	EEEE 70	HIS	2.6414	0.2451	4.2389
	EEEE 71	GLN	9.7531	6.2755	12.5353
	EEEE 72	GLN	15.3796	6.7847	22.2555
10	EEEE 73	VAL	6.0006	2.3479	10.8709
	EEEE 74	ASN	7.6007	0.9858	14.2156
	EEEE 75	GLU	9.6042	4.4474	13.7297
	EEEE 76	SER	0.6746	1.0066	0.0106
15	EEEE 77	GLU	12.7067	1.2232	21.8935
15	EEEE 78	PRO	2.3956	1.5978	3.4593
	EEEE 79	VAL	6.0444	0.7862	13.0553
	EEEE 80	TYR	4.1212	1.3782	5.4928
	EEEE 81 EEEE 82	LEU	0.4531	0.0000	0.9061
20		GLU	5.5155	0.0000	9.9279
20	EEEE 83 EEEE 84	VAL PHE	1.5309	2.6784	0.0008
	EEEE 85	SER	2.8834	0.6355	4.1679
	EEEE 86	ASP	11.0911	6.1575	20.9584
	EEEE 87	TRP	6.4143 9.2857	2.5687	10.2598
25	EEEE 88	LEU	9.2657 0.0519	0.2426 0.1037	12.9030
	EEEE 89	LEU	0.1205	0.0000	0.0000
	EEEE 90	LEU	0.0000	0.0000	0.2410 0.0000
	EEEE 91	GLN	0.2686	0.0000	0.4835
	EEEE 92	ALA	0.0943	0.0991	0.4633
30	EEEE 93	SER	4.2341	2.9403	6.8217
	EEEE 94	ALA	8.4724	1.4590	36.5259
	EEEE 95	GLU	4.3753	1.4778	6.6933
	EEEE 96	VAL	4.5984	4.5523	4.6599
	EEEE 97	VAL	1.5521	0.9731	2.3241
35	EEEE 98	MET	14.3494	0.0687	28.6301
	EEEE 99	GLU	7.4147	5.0436	9.3116
	EEEE 100	GLY	5.3477	5.3477	0.0000
	EEEE 101	GLN	9.6429	0.0120	17.3476
40	EEEE 102	PRO	9.4892	1.6653	19. 9211
40	EEEE 103 EEEE 104	LEU	0.0234	0.0192	0.0275
	EEEE 104 EEEE 105	PHE	6.1968	0.0000	9.7379
	EEEE 106	LEU ARG	0.0865	0.0657	0.1072
	EEEE 107	CYS	2.2169 0.6436	0.0000	3.4838
45	EEEE 108	HIS	1.1724	0.9654	0.0000
	EEEE 109	GLY	1.2996	0.2409 1.2996	1.7935
	EEEE 110	TRP	4.6388	0.3429	0.0000
	EEEE 111	ARG	14.4865	6.9035	6.3572 18.8197
	EEEE 112	ASN	13.2482	4.3960	22.1003
50	EEEE 113	TRP	7.0238	3.3035	8.5119
	EEEE 114	ASP	11.8883	1.9586	21.8181
	EEEE 115	VAL	0.8842	0.7257	1.0956
	EEEE 116	TYR	6.0204	0.0000	9.0306
	EEEE 117	LYS	11.3486	0.7247	19.8476
55	EEEE 118	VAL	0.0000	0.0000	0.0000
	EEEE 119	ILE	4.3850	. 0.0000	8.7700

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	EEEE 120	TYR	0.0002	0.0005	0.0000
	EEEE 121	TYR	3.8442	0.0044	5.7642
	EEEE 122	LYS	4.0492	0.9747	6.5088
_	EEEE 123	ASP	10.6363	6.3573	14.9153
5	EEEE 124	GLY	14.2853	14.2853	0.0000
	EEEE 125	GLU	13.3618	0.4051	23.7272
	EEEE 126	ALA	14.6809	5.6541	50.7878
	EEEE 127	LEU	9.2613	6.4361	12.0866
	EEEE 128	LYS	11.7127	1.6189	19.7878
10	EEEE 129	TYR	10.5042	5.1382	13.1872
	EEEE 130	TRP	8.3076	1.0723	11.2017
	EEEE 131	TYR	12.1072	0.8991	17.7113
	EEEE 132	GLU	12.7199	2.0028	21.2936
1.5	EEEE 133	ASN	5.6925	5.5621	5.8228
15	FFEE 134	HIS	8.1921	1.5201	12.6401
	EEEE 135	ASN	1.3201	0.2942	2.3461
	EEEE 136	ILE	2.2145	1.3058	3.1231
	EEEE 137	SER	10.0571	7.3406	15.4902
20	EEEE 138	ILE	3.4381	0.9086	5.9677
20	EEEE 139	THR	15.7625	2.5279	33.4087
	EEEE 140	ASN	6.4209	3.6811	9.1607
	EEEE 141	ALA	0.0000	0.0000	0.0000
	EEEE 142	THR	7.2538	0.3369	16.4763
25	EEEE 143	VAL	5.2826	1.1302	10.8192
25	EEEE 144 EEEE 145	GLU	14.2599	4.2746	22.2482
	EEEE 146	ASP	4.3200	0.0534	8.5866
	EEEE 147	SER GLY	5.5098	4.0762	8.3771
	EEEE 148	THR	2.9433	2.9433	0.0000
30	EEEE 149	TYR	5.7039	0.0995	13.1764
50	EEEE 150	TYR	0.2552	0.0130	0.3763
	EEEE 151	CYS	3.8275 0.0000	0.0000	5.7413
	EEEE 152	THR	3.7660	0.0000	0.0000
	EEEE 153	GLY	1.1095	0.0000 1.1095	8.7874
35	EEEE 154	LYS	6.0705	0.0037	0.0000
	EEEE 155	VAL	0.4853	0.0000	10.9239
	EEEE 156	TRP	11.8745	5.3337	1.1323 14.4908
	EEEE 157	GLN	14.3320	3.3004	23.1573
	EEEE 158	LEU	13.6525	0.2539	27.0512
40	EEEE 159	ASP	14.3336	5.0741	23.5931
	EEEE 160	TYR	3.5095	2.3905	4.0689
	EEEE 161	GLU	13.4677	5.2742	20.0225
	EEEE 162	SER	1.1284	1.6927	0.0000
	EEEE 163	GLU	9.6823	0.5318	17.0027
45	EEEE 164	PRO	10.3139	1.5274	22.0292
	EEEE 165	LEU	1.6379	0.1485	3.1273
	EEEE 166	ASN	3.3639	0.7774	5.9503
	EEEE 167	ILE	0.5534	1.0911	0.0157
	EEEE 168	THR	3.6331	0.0674	8.3873
50	EEEE 169	VAL	0.0817	0.1078	0.0468
	EEEE 170	ILE	2.1648	0.0777	4.2519
	EEEE 171	LYS	14.9019	13.4622	16.0537
	EEEE 221	NAG	13.0723	0.0000	13.0723
	EEEE 222	NAG	20.3453	0.0000	20.3453
55	EEEE 242	NAG	8.8452	0.0000	8.8452
	EEEE 243	NAG	7.6625	0.0000	7.6625

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	EEEE 244	MAN	18.6073	0.0000	18.6073
	EEEE 250	NAG	16.1217	0.0000	16.1217
	EEEE 274	NAG	22.0349	0.0000	22.0349
	EEEE 335	NAG	15.0552	0.0000	15.0552
5	EEEE 340	NAG	17,7238	0.0000	17.7238
	EEEE 366	NAG	12.1825	0.0000	12.1825
	EEEE 367	NAG	19.5820	0.0000	19 5820

Table 11. PhFc ϵ RI α_{1-176} , Form M2, residue exposure

>>>> coordinate set= md6c1.pdb

	segid	resid	resname	access	access-main	access-side
5	AAAA	1	VAL	23.3378	10.2131	40.8375
	AAAA	2	PRO	11.8969	4.7510	21.4247
	AAAA	3	GLN	4.0040	0.6188	6.7120
	AAAA	4	LYS	10.6487	3.0641	16.7164
	AAAA	5	PRO	0.2700	0.1467	0.4343
10	AAAA	6	LYS	14.5164	0.1128	26.0393
	AAAA	7	VAL	2.0175	3.5306	0.0002
	AAAA	8	SER	8.4156	1.5950	22.0570
	AAAA	9	LEU	3.4044	3.6981	3.1106
	AAAA	10	ASN	11.5698	0.5893	22.5503
15	AAAA	11	PRO	8.5175	0.1465	19.6787
	AAAA	12	PRO	9.1363	1.5259	19.2835
	AAAA	13	TRP	2.0981	0.0033	2.9360
	AAAA	14	ASN	2.7536	0.0000	5.5073
	AAAA	15	ARG	0.7887	0.0000	1.2394
20	AAAA	16	ILE	0.5825	0.0000	1.1649
	AAAA	17	PHE	0.1853	0.0000	0.2912
	AAAA	18	LYS	9.6106	1.2098	16.3312
	AAAA	19	GLY	4.3200	4.3200	0.0000
	AAAA	20	GLU	2.6272	0.0000	4.7290
25	AAAA	21	ASN	4.7245	2.9284	6.5206
	AAAA	22	VAL	0.4741	0.6955	0.1788
	AAAA	23	THR	4.7669	0.0001	11.1226
	AAAA	24	LEU	0.0001	0.0000	0.0002
	AAAA	25	THR	5.8774	0.0006	13.7131
30	AAAA	26	CYS	1.2474	1.8711	0.0000
	AAAA	27	ASN	9.8972	1.4492	18.3453
	AAAA	28	GLY	11.8125	11.8125	0.0000
	AAAA	29	ASN	10.4976	5.7985	15.1967
	AAAA	30	ASN	17.1596	4.7289	29.5903
35	AAAA	31	PHE	14.9024	9.0487	18.2474
	AAAA	32	PHE	6.9262	1.1011	10.2548
	AAAA	33	GLU	19.3638	7.9005	28.5344
	AAAA	34	VAL	10.5040	9.2873	12.1262
	AAAA	35	SER	20.0797	11.1239	37.9912
40	AAAA	36	SER	10.3115	2.5541	25.8262
	AAAA	37	THR	0.3123	0.1509	0.5275
	AAAA	38	LYS	9.1055	0.0303	16.3656
	AAAA	39	TRP	0.0125	0.0004	0.0173
	AAAA	40	PHE	3.3329	0.0507	5.2085
45	AAAA	41	HIS	3.3604	0.4369	5.3093
	AAAA	42	ASN	5.7196	5.9748	5.4644
	AAAA	43	GLY	11.0441	11.0441	0.0000
	AAAA	44	SER	12.3468	1.6054	33.8295
	AAAA	45	LEU	12.4194	6.6727	18.1661
50	AAAA	46	SER	6.2970	3.5164	11.8583
	AAAA	47	GLU	19.2754	6.3506	29.6153
	AAAA	48	GLU	5.5497	2.2183	8.2149
	AAAA	49	THR	10.8597	1.3240	23.5740

	AAAA	50	ASN	12.0836	1.0849	23.0822
	AAAA	.51	SER	8.5667	0.8380	24.0243
	AAAA	52	SER	6.5795	0.5607	18.6170
	AAAA	53	LEU	2.0088	0.0000	4.0175
5	AAAA	54	ASN	10.4631	4.8106	16.1155
	AAAA	55	ILE	1.5373	1.3922	1.6825
	AAAA	56	VAL	9.8664	4.5674	16.9318
	AAAA	57	ASN	8.3728	1.0485	15.6970
	AAAA	58	ALA	0.1673	0.2091	0.0000
10	AAAA	59	LYS	12.7698	0.0135	22.9748
	AAAA	60	PHE	2.9685	0.0000	4.6647
	AÀAA	61	GLU	10.1438	0.3798	17.9550
	AAAA	62	ASP	3.8187	0.0000	7.6375
	AAAA	63	SER	0.0423	0.0002	0.1265
15	AAAA	64	GLY	0.7550	0.7550	0.0000
	AAAA	65	GLU	4.0298	0.0243	7.2343
	AAAA	66	TYR	0.5144	0.0000	0.7716
	AAAA	67	LYS	4.6070	0.0021	8.2910
20	AAAA	68	CYS	0.0643	0.0965	0.0000
20	AAAA	69	GLN	4.3129	0.5930	7.2889
	AAAA	70	HIS	2.2107	1.4131	2.7425
	AAAA	71	GLN	15.8607	4.7123	24.7794
	AAAA	72	GLN	10.1949	4.9757	14.3702
25	AAAA	73	VAL	4.5886	3.4088	6.1618
23	AAAA AAAA	74	ASN	7.2228	1.6554	12.7903
	AAAA	75 76	GLU	11.1970	3.1686	17.6196
	AAAA	77	SER GLU	0.7529	1.1293	0.0000
	AAAA	78	PRO	5.6624	0.5155	9.7799
30	AAAA	79	VAL	9.4668	4.0586	16.6776
50	AAAA	80	TYR	4.2206 10.8696	0.7903	8.7943
	AAAA	81	LEU	0.3295	1.6448	15.4820
	AAAA	82	GLU	6.5599	0.6590 0.0000	0.0000
	AAAA	83	VAL	1.2313	2.1548	11.8078
35	AAAA	84	PHE	2.6783	1.0628	0.0000
	AAAA	85	SER .	10.4042	7.2453	3.6015 16.7222
	AAAA	86	ASP	6.7155	3.1365	10.7222
	AAAA	87	TRP	7.9670	0.0000	11.1538
	AAAA	88	LEU	0.2303	0.4605	0.0000
40	AAAA	89	LEU	0.1824	0.0005	0.3643
	AAAA	90	LEU	0.0000	0.0000	0.0000
	AAAA	91	GLN	0.1542	0.0000	0.2776
	AAAA	92	ALA	0.0000	0.0000	0.0000
	AAAA	93	SER	6.4731	4.6474	10.1245
45	AAAA	94	ALA	6.9800	1.7371	27.9520
	AAAA	95	GLU	6.3625	0.8834	10.7457
	AAAA	96	VAL	12.7032	5.5496	22.2413
	AAAA	97	VAL	1.4127	0.9895	1.9769
	AAAA	98	MET	8.3663	0.9908	15.7417
50	AAAA	99	GLU	6.0466	3.8025	7.8419
	AAAA	100		1.3823	1.3823	0.0000
	AAAA	101	GLN	9.3401	0.0000	16.8122
	AAAA	102	PRO	11.5211	1.3350	25.1025
	AAAA	103	LEU	0.2239	0.2968	0.1510
55	AAAA	104	PHE	5.5960	0.0000	8.7937
	AAAA	105	LEU	. 0.2800	. 0.0000	0.5599

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	AAAA	106	ARG	5.6019	0.0000	8.8030
	AAAA	107	CYS	1.9041	2.6369	0.4387
	AAAA	108	HIS	1.2459	0.8447	1.5133
	AAAA	109	GLY	0.2958	0.2958	0.0000
5	AAAA	110	TRP	3.6776	0.2682	5.0414
	AAAA	111	ARG	13.9748	6.0118	18.5251
	AAAA	112	ASN	13.0426	5.9312	20.1540
	AAAA	113	TRP	8.4374	2.2626	10.9073
	AAAA	114	ASP	10.8862	0.8382	20.9341
10	AAAA	115	VAL	3.6736	4.0353	3.1913
	AAAA	116	TYR	10.8526	0.9359	15.8110
	AAAA	117	LYS	12.5729	4.0303	19.4070
	AAAA	118	VAL	1.5367	1.4181	1.6949
	AAAA	119	ILE	3.8886	0.4794	7.2979
15	AAAA	120	TYR	0.1235	0.0400	0.1653
	AAAA	121	TYR	3.2159	0.0000	4.8238
	AAAA	122	LYS	4.1348	0.5235	7.0239
	AAAA	123	ASP	9.0341	4.7242	13.3440
20	AAAA	124	GLY	12.8886	12.8886	0.0000
20	AAAA	125	GLU	13.5568	0.5821	23.9366
	AAAA	126	ALA	5.4448	3.6508	12.6207
	AAAA	127	LEU	4.4392	1.2148	7.6637
	AAAA	128	LYS	6.6847	0.4089	11.7054
25	AAAA	129	TYR	17.7661	6.5522	23.3730
23	AAAA AAAA	130	TRP	4.6781	0.2956	6.4311
	AAAA	131 132	TYR	5.9070	2.3743	7.6733
	AAAA	133	GLU ASN	14.4146	6.3584	20.8595
	AAAA	134	HIS	9.2636	0.7631	17.7642
30	AAAA	135	ASN	14.3143	1.4912	22.8630
50	AAAA	136	ILE	6.6861 0.1409	0.2683	13.1040
	AAAA	137	SER	9.4451	0.0100 3.2255	0.2719
	AAAA	138	ILE	2.6491	0.8829	21.8842 4.4154
	AAAA	139	THR	12.8859	1.4417	28.1448
35	AAAA	140	ASN	6.4432	3.5706	9.3157
	AAAA	141	ALA	1.3406	1.6757	0.0000
	AAAA	142	THR	7.2752	0.0020	16.9727
	AAAA	143	VAL	11.7608	1.2461	25.7803
	AAAA	144	GLU	14.7507	2.5626	24.5012
40	AAAA	145	ASP	3.5866	0.0546	7.1186
	AAAA	146	SER	4.2659	2.0709	8.6561
	AAAA	147	GLY	2.4870	2.4870	0.0000
	AAAA	148	THR	3.9797	0.0000	9.2860
	AAAA	149	TYR	0.3266	0.0000	0.4899
45	AAAA	150	TYR	3.1527	0.0005	4.7289
	AAAA	151	CYS	0.0003	0.0005	0.0000
•	AAAA	152	THR	4.1824	0.6979	8.8283
	AAAA	153	GLY	0.7331	0.7331	0.0000
	AAAA	154	LYS	7.5163	0.0133	13.5188
50	AAAA	155	VAL	0.2906	0.0000	0.6781
	AAAA	156	TRP	11.8912	1.7474	15.9487
	AAAA	157	GLN	14.6241	5.4565	21.9582
	AAAA	158	LEU	13.5291	0.9340	26.1242
	AAAA	159	ASP	14.3755	5.4004	23.3507
55	AAAA	160	TYR	3.1668	2.6149	3.4428
	AAAA	161	GLU	10.8144	4.2630	16.0556

	AAAA AAAA	162 163	SER GLU	0.5614 10.6063	0.8334 0.2900	0.0172
	AAAA	164	PRO	10.9414	3.3661	18.8593
	AAAA	165	LEU	1.9287	0.7267	21.0417
5	AAAA	166	ASN	5.8142	3.0970	3.1308
•	AAAA	167	ILE	0.2918	0.5835	8.5314
	AAAA	168	THR	9.3327	0.0000	0.0000
	AAAA	169	VAL	0.2835	0.4961	21.7764
	AAAA	170	ILE	10.1702	0.5659	0.0000
10	AAAA	171	LYS	14.8660	3.9580	19.7745
	AAAA	172	ALA	10.1636	3.7167	23.5925
	AAAA	173	PRO	16.8141	8.4692	35.9516
	AAAA	174	ARG	24.7335	21.3158	27.9405
	AAAA	221	NAG	10.3017	0.0000	26.6865 10.3017
15	AAAA	222	NAG	20.4990	0.0000	20.4990
	AAAA	242	NAG	10.4998	0.0000	10.4998
	AAAA	243	NAG	9.1915	0.0000	
	AAAA	244	MAN	17.0951	0.0000	9,1915
	AAAA	274	NAG	8.2536	0.0000	17.0951
20	AAAA	275	FCA	13.5116	0.0000	8.2536
	AAAA	276	NAG	18.0492	0.0000	13.5116
	AAAA	340	NAG	18.2117	0.0000	18.0492
	AAAA	366	NAG	20.2201	0.0000	18.2117
	BBBB	1	VAL	23.2202	13.0224	20.2201
25	BBBB	2	PRO	12.9287	6.5376	36.8172
	BBBB	3	GLN	7.8969	1.1767	21.4502 13.2731
	BBBB	4	LYS	10.9639	2.4069	
	BBBB	5	PRO	0.1485	0.1774	17.8095
	BBBB	6	LYS	13.6900	0.3136	0.1101
30	BBBB	7	VAL	2.0335	3.5586	24.3911 0.0000
	BBBB	8	SER	8.6515	1.6168	22.7209
	BBBB	9	LEU	3.3843	3.6519	3.1168
	BBBB	10	ASN	11.2166	0.5892	21.8441
	BBBB	11	PRO	6.4967	0.0774	15.0558
35	BBBB	12	PRO	5.5258	1.4792	10.9213
	BBBB	13	TRP	0.5399	0.0000	0.7559
	BBBB	14	ASN	2.8551	0.0000	5.7102
	BBBB	15	ARG	0.8228	0.0000	1.2930
	BBBB	16	ILE	0.7004	0.0000	1.4007
40	BBBB	17	PHE	0.2062	0.0000	0.3240
	BBBB	18	LYS	10.1266	2.4178	16.2937
	BBBB	19	GLY	5.1193	5.1193	0.0000
	BBBB	20	GLU	3.6592	0.0000	6.5866
	8888	21	ASN	4.9980	2.8696	7.1265
45	BBBB	22	VAL	0.3086	0.5358	0.0056
	BBBB	23	THR	4.8914	0.0060	11.4053
	8888	24	LEU	0.0000	0.0000	0.0000
	BBBB	25	THR	5.3161	0.0000	12.4043
	BBBB	26	CYS	1.7698	1.9470	1.4152
50	BBBB	27	ASN	9.5595	2.4594	16.6596
	BBBB	28	GLY	5.1022	5.1022	0.0000
	BBBB	29	ASN	11.6239	9.1902	14.0577
	BBBB	30	ASN	11.1354	7.5265	14.0577
	BBBB	31	PHE	12.4823	0.9411	19.0773
55	BBBB	32	PHE	14.9629	4.4534	20.9683
	BBBB	33	GLU	10.0579	1.1430	17.1898
		_		. 5.55. 5		17.1090

	BBBB	34	VAL	8.1169	2.1335	16.0948
	BBBB	.35	SER	17.2091	9.6972	32.2329
	BBBB	36	SER	5.6660	1.8677	13.2627
	8888	37	THR	0.9190	0.7693	1.1187
5	BBBB	38	LYS	10.5493	0.0585	18.9418
	BBBB	39	TRP	0.0160	0.0000	0.0224
	BBBB	40	PHE	3.2085	0.1128	4.9774
	BBBB	41	HIS	3.2674	0.7993	4.9129
	BBBB	42	ASN	6.9206	7.0588	6.7824
10	BBBB	43	GLY	10.5521	10.5521	0.0000
	BBBB	44	SER	12.5873	1.8007	34.1606
	BBBB	45	LEU	12.5684	7.0671	18.0697
	BBBB	46	SER	5.8736	2.9025	11.8159
1.5	BBBB	47	GLU	18.2898	4.6076	29.2356
15	BBBB	48	GLU	6.4732	2.2413	9.8587
	BBBB	49	THR	12.4950	1.2186	27.5 302
	BBBB	50	ASN	10.6353	1.9696	19.3010
	BBBB	51	SER	2.7922	0.0131	8.3506
20	BBBB	52	SER	5.4540	0.4267	15.5085
20	BBBB	53	LEU	2.2138	0.0004	4.4271
	BBBB	54	ASN	10.5005	4.6511	16.3499
	BBBB	55	ILE	1.3385	1.1102	1.5667
	BBBB	56	VAL	11.5067	3.9707	21.5548
25	BBBB	57	ASN	8.7141	1.1097	16.31 85
25	BBBB	58	ALA	0.1840	0.2300	0.0000
	BBBB	59	LYS	13.0236	0.0000	23.4424
	BBBB	60	PHE	2.3308	0.0000	3.6627
	BBBB	61	GLU	9.4233	0.1906	16.8095
30	BBBB	62	ASP	3.8339	0.0000	7.6678
30	BBBB	63	SER	0.1605	0.0000	0.4815
	BBBB	64	GLY	1.6421	1.6421	0.0000
	8888 8888	65	GLU	3.9224	0.0377	7.0302
	8888	66	TYR	0.5105	0.0000	0.7658
35		67	LYS	3.9749	0.0002	7.1547
JJ	8888 8888	68 69	CYS	0.0929	0.1393	0.0000
	BBBB	70	GLN HIS	5.4367	0.1443	9.6707
	BBBB	71		4.9806	0.9868	7.6431
	BBBB	72	GLN GLN	14.5333	5.4826	21.7740
40	BBBB	73	VAL	18.4063	11.6333	23.8247
70	BBBB	74	ASN	2.6548	3.2121	1.9118
	8888	7 4 75	GLU	12.0029	2.0287	21.9770
	BBBB	76	SER	8.4921	2.6890	13.1345
	BBBB	70 77	GLU	0.7254 7.7802	1.0881	0.0000
45	BBBB	78	PRO	9.3860	0.6132	13.5138
15	BBBB	79	VAL	4.0363	3.7419	16.9114
	BBBB	80	TYR	4.0363 11.1782	0.8626	8.2679
	BBBB	81	LEU	0.2983	1.6916	15.9215
	BBBB	82	GLU	7.4968	0.5965	0.0000
50	BBBB	83	VAL	1.2876	0.0000	13.4942
	BBBB	84	PHE	2.7723	2.2532	0.0000
	8888	85	SER	10.1939	1.0285	3.7688
	BBBB	86	ASP	6.5079	7.3007	15.9804
	BBBB	87	TRP	6.1336	3.0391	9.9768
55	BBBB	88	LEU	0.2766	0.0000 0.5478	8.5870
	BBBB	89	LEU	0.2222		0.0054
		39	LLU	U.ZZZZ	0.0049	0.4394

	BBBB	90	LEU	0.0152	0.0302	0.0001
	BBBB		GLN	0.1468	0.0000	0.2642
	BBBB		ALA	0.0005	0.0006	0.0000
_	BBBB		SER	5.6156	4.5602	7.7265
5	BBBB		ALA	6.8297	1.8546	26.7302
	BBBB		GLU	6.8738	0.8762	11.6719
	BBBB	96	VAL	12.2316	5.3212	21.4456
	BBBB	97	VAL	1.4488	1.1013	1.9123
10	BBBB	98	MET	11.2447	0.4365	22.0530
10	8888	99	GLU	6.9392	5.4744	8.1110
	BBBB	100	GLY	2.1371	2.1371	0.0000
	BBBB	101	GLN	10.3142	0.0031	18.5631
	BBBB	102	PRO	10.9007	1.3692	23.6094
15	BBBB	103	LEU	0.1806	0.2907	0.0705
13	BBBB	104	PHE	0.9676	0.0002	1.5204
	8888 8888	105 106	LEU	0.2088	0.0016	0.4161
	BBBB	107	ARG	3.6986	0.0002	5.8119
	BBBB	108	CYS HIS	0.0292	0.0438	0.0000
20	BBBB	109	GLY	1.4195	0.6184	1.9535
20	BBBB	110	TRP	0.5887	0.5887	0.0000
	BBBB	111	ARG	0.8590	0.0000	5.4025
	BBBB	112	ASN	12.1336 13.9325	6.9873	15.0744
	BBBB	113	TRP	3.3478	3.3709 2.2053	24.4942
25	BBBB	114	ASP	7.6950		3.8048
	BBBB	115	VAL	0.1840	3.0188 0.2489	12.3711
	BBBB	116	TYR	4.9222	0.0000	0.0975 7.3832
	BBBB	117	LYS	10.4451	0.8887	18.0902
	BBBB	118	VAL	0.0000	0.0000	0.0000
30	BBBB	119	ILE	4.6639	0.0004	9.3274
	BBBB	120	TYR	0.0002	0.0000	0.0003
	BBBB	121	TYR	3.8872	0.0000	5.8308
	BBBB	122	LYS	4.3212	0.6213	7.2812
	BBBB	123	ASP	9.3317	5.1768	13.4866
35	BBBB	124	GLY	14.0149	14.0149	0.0000
	BBBB	125	GLU	14.1323	1.6253	24.1378
	BBBB	126	ALA	12.2018	6.3993	35.4121
	BBBB	127	LEU	9.7819	5.9893	13.5746
40	BBBB	128	LYS	10.6006	2.2370	17.2915
40	BBBB	129	TYR	9.1175	4.6166	11.3680
	BBBB	130	TRP	11.8627	0.8908	16.2515
	BBBB	131	TYR	9.3270	0.4323	13.7744
	BBBB	132	GLU	10.1438	0.0000	18.2588
45	BBBB	133	ASN	4.9699	1.6521	8.2877
43	BBBB	134	HIS	2.1605	0.1201	3.5207
	BBBB	135	ASN	3.4385	4.8744	2.0027
	8888 8888	136	ILE	0.1878	0.2608	0.1149
	BBBB	137 138	SER	10.4452	5.0394	21.2570
50	BBBB	139		4.4124	0.8988	7.9260
50	8888	140	THR	13.3105	0.5909	30.2701
	BBBB	141	ASN ALA	6.8155	3.1228	10.5082
	BBBB	142	THR	1.3398 7.5421	1.6747	0.0000
	BBBB	143	VAL	7.5 4 21 11.6452	0.0097	17.5852
55	BBBB	144	GLU	14.1708	1.2806	25.4646
	BBBB	145	ASP	3.4895	1.1173 . 0.0584	24.6136
			,,	0.4030	. 0.0564	6.9206

	BBBB	146	SER	4.2945	1.9825	0.0404
	BBBB	. 147	GLY	4.2945 4.3457	4.3457	8.9184
	BBBB	148	THR	4.3457 4.4415	0.0000	0.0000
	BBBB	149	TYR		0.0000	10.3634
5	BBBB	150	TYR	0.0214 3.1691	0.0001	0.0321
3	BBBB					4.7537
	B888	151 152	CYS	0.0000	0.0000	0.0000
	8888	153	THR GLY	3.5053	0.0000	8.1791
		154		0.6931	0.6931	0.0000
10	BBBB		LYS	6.3103	0.0180	11.3441
10	BBBB	155	VAL	0.0365	0.0044	0.0793
	BBBB	156	TRP	3.3899	5.9121	2.3810
	BBBB	157	GLN	16.5870	5.2100	25.6886
	BBBB	158	LEU	13.1911	0.1922	26.1899
1.5	BBBB	159	ASP	13.0965	5.2133	20.9797
15	BBBB	160	TYR	3.2939	3.1627	3.3595
	BBBB	161	GLU	10.8490	4.6790	15.7851
	BBBB	162	SER	0.5960	0.7781	0.2318
	BBBB	163	GLU	10.5937	0.3366	18.7993
••	BBBB	164	PRO	11.6713	3.2190	22.9411
20	BBBB	165	LEU	1.9716	0.7957	3.1476
	BBBB	166	ASN	5.2287	2.2398	8.2176
	BBBB	167	ILE	0.2784	0.5568	0.0000
	BBBB	168	THR	9.3922	0.0000	21.9152
	BBBB	169	VAL	0.2895	0.5066	0.0000
25	BBBB	170	ILE	9.7952	0.6056	18.9 848
	BBBB	171	LYS	14.9992	3.9650	23.8265
	BBBB	172	ALA	8.6682	3.2571	30.3128
	BBBB	173	PRO	17.2332	8.4405	28.9567
	BBBB	174	ARG	24.5074	21.0894	26.4605
30	BBBB	221	NAG	17.4850	0.0000	17.4850
	BBBB	242	NAG	10.4355	0.0000	10.4355
	BBBB	243	NAG	10.3502	0.0000	10.3502
	BBBB	244	MAN	15.8885	0.0000	15.8885
	BBBB	335	NAG	8.8279	0.0000	8.8279
35	BBBB	336	NAG	16.5384	0.0000	16.5384
	BBBB	337	FCA	16.2107	0.0000	16.2107
	BBBB	340	NAG	13.5916	0.0000	13.5916
	BBBB	341	NAG	21.2819	0.0000	21.2819
	BBBB	366	NAG	21.9238	0.0000	21.9238

Table 12. PhFc ϵ RI α_{1-172} , Form H1, residue exposure

>>>> coordinate set= c703f.pdb

	segid		فيرير <u>ة</u>	qe accessible a	ırea
	<u>sidechain</u>	resid	resname	residue	mainchain
5	1	VAL	22.5900	15.0637	32.6251
	2	PRO	11.2478	3.9295	21.0055
	3	GLN	15.8860	3.9559	25.4300
	4	LYS	7.8658	4.1508	10.8378
	5	PRO	0.7859	0.7412	0.8456
10	6	LYS	15.0743	0.2689	26.9185
	7	VAL	2.5158	4.4026	0.0000
	8	SER	8.7041	1.7476	22.6170
	9	LEU	3.4804	4.2930	2.6678
	10	ASN	13.3748	1.0394	25.7103
15	11	PRO	6.4372	0.6223	14.1904
15	12	PRO	9.9906	1.9726	20.6812
	13	TRP	1.6444	0.0463	2.2837
	14	ASN	2.4971	0.0178	4.9764
	15	ARG	1.2172	0.0001	1.9127
20	16	ILE	0.3947	0.0000	0.7895
20	17	PHE	0.1203	0.0000	0.1890
	18	LYS	9.6134	1.5661	16.0512
	19	GLY	6.4465	6.4465	0.0000
	20	GLU	2.9946	0.0000	5.3903
25	21	ASN	4.7501	2.8416	6.6586
2.5	22	VAL	0.3670	0.6423	0.0000
	23	THR	5.0060	0.1082	11.5364
	23 24	LEU	0.2483	0.0000	0.4966
	2 4 25	THR	4.0121	0.0000	9.3616
30	26 26	CYS		0.1881	
30	20 27	ASN	0.1821 6.6425	2.1781	0.1702 11.1069
	28	GLY	5.3679	5.3679	0.0000
	29	ASN	17.4099	6.2098	
					28.6100
25	30	ASN	10.2762	3.8525	16.6998
35	31	PHE	8.0955	2.8330	11.1027
	32	PHE	13.6377	6.1749	17.9021
	33	GLU	14.0698	3.4930	22.5313
	34	VAL	17.4046	4.8614	34.1288
40	35	SER	19.6721	12.8131	33.3901
40	36	SER	11.0819	4.5899	24.0659
	37	THR	0.8916	0.1902	1.8268
	38	LYS	8.3803	0.0158	15.0719
	39	TRP	0.0119	0.0000	0.0167
45	40	PHE	3.9461	0.0636	6.1646
45	41	HIS	3.7169	0.6731	5.7461
	42	ASN	6.6160	8.2911	4.9408
	43	GLY	11.9937	11.9937	0.0000
	44	SER	11.8169	1.4187	32.6133
	45	LEU	12.1877	6.2251	18.1503
50	46	SER	4.5272	3.1407	7.3002
	47	GLU	18.3989	5.5809	28.6533
	48	GLU	1.6700	0.3535	2.7232

	49	THR	6.8437	0.4232	15.4044
	50	ASN	6.1820	1.4496	10.9145
	51	SER	8.4271	1.0315	23.2182
_	52	SER	6.0403	0.9347	16.2516
5	53	LEU	1.9666	0.0000	3.9331
	54	ASN	10.6560	4.7155	16.5965
	55	ILE	1.5407	1.0849	1.9965
	56	VAL	8.4966	4.2813	14.1170
4.0	57	ASN	8.0710	0.2994	15.8427
10	58	ALA	0.4475	0.5594	0.0000
	59	LYS	12.6628	0.0000	22.7931
	60	PHE	2.0470	0.0207	3.2050
	61	GLU	9.1096	0.1120	16.3076
. ~	62	ASP	3.9382	0.0000	7.8765
15	63	SER	0.1178	0.0000	0.3535
	64	GLY	0.5477	0.5477	0.0000
	65	GLU	3.5925	0.1947	6.3107
•	66	TYR	0.3061	0.0000	0.4592
00	67	LYS	4.9263	0.0000	8.8674
20	68	CYS	0.0002	0.0002	0.0000
	69	GLN	3.1065	0.1191	5.4965
	70	HIS	4.3287	0.5494	6.8482
	71	GLN	14.4511	4.6243	22.3126
25	72 	GLN	16.7254	5.5984	25.6271
25	73	VAL	4.6849	0.0239	10.8997
	74	ASN	3.7390	2.2152	5.2628
	75 70	GLU	9.8220	1.6123	16.3897
	<u>76</u>	SER	0.9279	1.3599	0.0638
20	77 70	GLU	10.2035	0.8100	17.7182
30	78 70	PRO	6.8952	4.7323	9.7791
	79	VAL	4.4704	0.8249	9.3311
	80	TYR	10.8485	1.3619	15.5919
	81	LEU	0.8740	1.0895	0.6586
35	82	GLU	6.2336	0.0000	11.2205
33	83	VAL	1.6724	2.9266	0.0000
	84 85	PHE	3.0301	0.8580	4.2712
	86	SER	10.9935	6.5698	19.8409
	87	ASP	6.6012	2.2575	10.9449
40		TRP	9.0703	0.2059	12.6161
40	88 89	LEU	0.4451	0.8570	0.0331
		LEU	0.5432	0.0676	1.0187
	90 91	LEU	0.0913	0.1298	0.0527
	91 92	GLN	0.0763	0.0000	0.1373
45	92 93	ALA SER	0.0388	0.0480	0.0022
45	93 94		4.5675	4.1995	5.3034
	95	ALA GLU	7.1276	1.0786	31.3237
	96	VAL	6.8795	1.2919	11.3495
	97	VAL	13.0247	4.2238	24.7593
50	98	MET	1.0770	0.5985	1.7150
50	99		16.7988	0.4914	33.1061
	100	GLU GLY	7.5393	3.3688	10.8758
	101	GLY	3.1157	3.1157	0.0000
	102	PRO	10.1587	0.2304	18.1014
55	103	LEU	8.7856 0.0405	1.4883	18.5154
<i>JJ</i>	104	PHE	0.0405 5.7300	0.0000	0.0810
	104	rnc	5.7390	0.0000	9.0184

			•		
	105	LEU	0.0000	0.0000	0.0000
	106	ARG	4.9770	0.0000	7.8210
	107	CYS	2.8329	3.8594	0.7800
	108	HIS	1.0226	0.3429	1.4757
5	109	GLY	0.7524	0.7524	0.0000
•	110	TRP	4.3881	0.0000	6.1433
	111	ARG	13.1221	5.0820	17.7164
	112	ASN	12.3893	5.7597	19.0188
	113	TRP	6.4754	2.8590	7.9219
10	114	ASP	11.2956	2.1441	20.4471
	115	VAL	2.0499	2.1826	1.8731
	116	TYR	11.1258	1.0112	16.1831
	117	LYS	16.7863	4.7622	26.4055
	118	VAL	8.1424	6.0958	10.8711
15	119	ILE	6.8012	0.9964	12.6060
	120	TYR	2.8442	0.9061	3.8133
	121	TYR	3.5867	0.0012	5.3794
	122	LYS	5.1214	0.6012	8.7376
	123	ASP	7.4941	4.6376	10.3507
20	124	GLY	12.2128	12.2128	0.0000
	125	GLU	15.1128	1.2362	26.2141
	126	ALA	11.6923	3.6139	44.0058
	127	LEU	4.6471	5.4019	3.8923
	128	LYS	18.8922	6.6649	28.6740
25	129	TYR	17.4834	7.0989	22.6757
	130	TRP	2.4961	4.3542	1.7528
	131	TYR	12.7233	5.2485	16.4608
	132	GLU	13.6661	0.7556	23.9944
	133	ASN	9.3922	6.3761	12.4084
30	134	HIS	15.2795	8.2917	19.9381
	135	ASN	11.1940	2.7459	19.6420
	136	ILE	5.4540	0.6821	10.2259 2.0744
	137	SER	0.6915	0.0000	
	138	ILE	6.3883	1.6352	11.1413 8.2152
35	139	THR	4.7987	2.2363	
	140	ASN	5.2615	2.7779	7.7451 0.0000
	141	ALA	0.9545	1.1931	15.3420
	142	THR	6.9219	0.6069	19.8448
	143	VAL	9.5663	1.8575	23.3579
40	144	GLU	14.4371	3.2860	4.4384
	145	ASP	2.2220	0.0056	11.3756
	146	SER	5.2393	2.1/12	0.0000
	147	GLY	3.0536	3.0536 0.0000	6.6250
	148	THR	2.8393	0.0000	0.0734
45	149	TYR	0.0489	0.0000	4.9500
	150	TYR	3.3061	0.0000	0.0000
	151	CYS	0.0000	0.0000	8.6679
	152	THR	3.7148	0.0000	0.0000
	153	GLY	0.9412	0.1238	15.0704
50	154	LYS	8.4275	0.1238	0.7223
	155	VAL	0.3174	7.2900	16.9477
	156	TRP	14.1884	7.2900 4.5161	24.2122
	157	GLN	15.4584	0.7276	22.3193
سر سع	158	LEU	11.5234 15.3714	7.3517	23.3910
55	159	ASP	4.5849	1.8192	5.9678
	160	TYR	4.3048	1.0192	0.0010

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			•		
	161	GLU	12.0528	4.8779	17.7927
	162	SER	0.9680	1.3220	0.2601
	163	GLU	10.9265	0.9944	18.8722
	164	PRO	11.4182	2.7638	22.9575
5	165	LEU	1.8797	0.4866	3.2727
_	166	ASN	5.1428	2.5621	7.7235
	167	ILE	0.3717	0.7433	0.0000
	168	THR	9.9155	0.0000	23.1363
	169	VAL	0.2713	0.4747	0.0000
10	170	ILE	12.6290	1.6535	23.6046
	171	LYS	18.1223	11.6928	23.2660
	221	NAG	10.3807	0.0000	10.3807
	222	NAG	20.2927	0.0000	20.2927
	242	NAG	10.3379	0.0000	10.3379
15	243	NAG	10.0051	0.0000	10.0051
	244	MAN	17.1981	0.0000	17.1981
	250	NAG	15.4600	0.0000	15.4600
	274	NAG	20.0516	0.0000	20.0516
	340	NAG	16.0149	0.0000	16.0149
20	341	NAG	20.8951	0.0000	20.8951
	366	NAG	14.4348	0.0000	14.4348
	367	NAG	20.6913	0.0000	20.6913

Table 13. Crystallographic data and model refinement

		500 (2)	Tomat .	Egme r 2
res.	3.2	3.2	3.1	3.8
wavel(A)	1.0039	1.0047	0.914	0.92
comp/(last shell)	93.2(95.4)	99.3(100)	97.0(83.3)	85.7(80.2)
av. red. (last shell)	8.0(7.1)	4.1(4.2)	7.3(2.2)	2.0(1.6)
Rmerge (last shell)	10.3(51.6)	9.7(43.6)	11.2(76.6)	6.3(60.9)
l/sigl (last shell)	11.8(5.3)	9.2(3.0)	7.9(1.1)	7.5(1.1)
#refl(free)	4030(412)	11640(620)	23318(1180)	14239(740)
Rfactor/Rfree	28.8/31.3	25.4/28.3	29.1/32.9	27.8/30.4
# atoms	1537	3120	7660	7660
# waters	0	0	0	0
RMSD bonds	0.0084	0.0096	0.0100	0.0086
RMSD angles	1.53	1.60	1.50	1.40
Ave. B	97.1	69.4	137.6	191.1

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Table 14. Root mean square deviations for alpha carbon positions

model.	FIMSO v. origi(Arigis)	#CA	septoepts T
Н1	0.855	155	4-27/28-31/36-70/73-129/137-17
H1 30 loop	3.667	6	27-31, 36
H1 130 loop	4.176	9	129-137
M2 copy A	0.880	157	4-27/36-130/134-171
M2A 30 loop	5.212	6	27-31, 36
M2A 130 loop	3.818	5	130-134
М2 сору В	0.766	155	4-27/36-127/133-171
M2B 30 loop	4.258	6	27-31, 36
M2B 130 loop	6.938	7	127-133 .
T1 copy C	0.839	155	4-28/36-71/73-127/133-171
T1C 30 loop	6.372	5	28-31, 36
T1C 130 loop	7.449	7	127-133
T2 copy C	0.867	155	4-28/36-71/73-127/133-171
T1C 30 loop	6.319	5	28-31, 36
T1C 130 loop	7.476	7	127-133

While various embodiments of the present invention have been described in detail, it is apparent that modifications and adaptations of those embodiments will occur to those skilled in the art. It is to be expressly understood, however, that such modifications and adaptations are within the scope of the present invention, as set forth in the following claims.

What is claimed is:

- 1. A three-dimensional model selected from the group consisting of: (a) a three-dimensional model of an extracellular domain of a human high affinity Fc epsilon receptor alpha chain (FceRla) protein, wherein said model substantially represents the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7, and Table 8; and (b) a three-dimensional model comprising a modification of said model of (a), wherein said modification represents a protein that binds to a Fc domain of an antibody.
- 2. A method to produce a three-dimensional model of an extracellular domain of a human FceRIa protein, said method comprising representing amino acids of said protein at substantially the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8.
- 3. A method to produce a three-dimensional model of an antibody receptor protein other than a human FceRIa protein represented by the three-dimensional model substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8, said method comprising homology modeling.
 - 4. An isolated crystal of an extracellular domain of a FceRIa protein.
- 5. A method to produce an isolated crystal of an extracellular domain of a FceRIa protein, said method comprising vapor diffusion.
- 6. An isolated FceRIa protein selected from the group consisting of: (a) a protein consisting of SEQ ID NO:2; (b) a protein consisting of SEQ ID NO:4 except that the isoleucine at position 170 is replaced with a cysteine; and (c) a protein that is structurally homologous to a protein of (a) or (b), wherein said protein of (c) binds to a Fc domain of an antibody.
- 7. A method to identify a compound that inhibits the binding between an IgE antibody and a FceRIa protein, said method comprising using a three-dimensional model of an extracellular domain of a human high affinity FceRIa protein to identify said compound, wherein said model substantially represents the atomic coordinates

specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8.

- 8. A mutein that binds to a Fc domain of an antibody, wherein said mutein has an improved function compared to a protein comprising an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4, wherein said improved function is selected from the group consisting of increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, wherein said mutein is produced by a method comprising:
 - (a) analyzing a three-dimensional model substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8 to identify at least one amino acid of the protein represented by said model which if replaced by a specified amino acid would effect said improved function of said protein; and
 - (b) replacing said identified amino acid(s) to produce said mutein having said improved function.
- 9. A mutein having an improved function compared to an unmodified FceRIa protein, wherein said improved function is selected from the group consisting of increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, wherein the amino acid sequence of said mutein differs in at least one position from the amino acid sequence of said unmodified protein, said position being in a region selected from the group consisting of a crystal contact cluster, a tryptophan-containing hydrophobic ridge, a FG loop in D2, a D1D2 interface, a cleft between D1 and D2, a domain 1, a domain 2, a hydrophobic core, a A'B loop of D1, a EF loop of D1, a BC loop of D2, a C strand of D2, a CC' loop of D2, a C'E loop of D2, a strand of D2, the amino terminal five residues of said protein, and the carboxyl terminal five residues of said protein.
- 10. A method to improve a function of a FceRIa protein, said improved function being selected from the group consisting of increased stability, increased affinity for an Fc domain of an antibody, altered substrate specificity, and increased solubility, said method comprising:

- (a) analyzing a three-dimensional model of an extracellular domain of a human high affinity FcεRIα protein substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8 to identify at least one amino acid of said protein which if replaced by a specified amino acid improves at least one of said functions of said protein; and
- (b) replacing said identified amino acid(s) to produce a mutein having at least one of said improved functions.
- 11. An isolated FceRIa protein selected from the group consisting of: a crystal contact cluster involved in IgE binding; a tryptophan-containing hydrophobic ridge; a FG loop in D2; a D1D2 interface; a cleft between D1 and D2; a domain 1; a domain 2; a hydrophobic core; a A'B loop of D1; a EF loop of D1; a BC loop of D2; a C strand of D2; a CC' loop of D2; a C'E loop of D2; and a strand of D2.
- 12. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model is represented by a method selected from the group consisting of listing the coordinates of all atoms comprising said model, providing a physical three-dimensional model, imaging said model on a computer screen, providing a picture of said model, and deriving a set of coordinates based of a picture of said model.
- 13. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model identifies the solvent accessibility of amino acid residues of said protein listed in a table selected from the group consisting of Table 2, Table 9, Table 10, Table 11 and Table 12.
- 14. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents a protein that binds to a Fc domain of an IgE antibody with an affinity that is at lesst equivalent to the affinity of the extracellular domain of human FcεRIα for an IgE antibody selected from the group consisting of a human IgE antibody, a canine IgF antibody, a feline IgE antibody, an equine IgE antibody, a rat IgE antibody, and a murine IgE antibody.
- 15. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents a protein that selectively binds to a mammalian antibody selected from the group consisting of an IgE antibody and an IgG antibody.

- 16. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents an extracellular domain of a protein selected from the group consisting of a human FceRIa protein, a canine FceRIa protein, a feline FceRIa protein, an equine FceRIa protein, a murine FceRIa protein, and a rat FceRIa protein.
- 17. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model comprises a three-dimensional model of an extracellular antibody binding domain of an antibody receptor protein other than human FceRIa.
- 18. The invention of Claim 17, wherein said model is produced by incorporating all or any part of the amino acid sequence of said other antibody receptor protein into a three-dimensional model of said extracellular domain of said human FceRIa protein to produce said model of said other antibody receptor protein.
- 19. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model represents an IgE binding domain.
- 20. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model is produced by a method comprising:
 - (a) crystallizing an extracellular domain of a human FceRIa protein;
 - (b) collecting X-ray diffraction data from said crystallized protein; and
 - (c) determining said model from said data and amino acid sequence of said protein.
- 21. The invention of Claim 20, wherein said protein has an amino acid sequence selected from the group consisting of SEQ ID NO:2, SEQ ID NO:4 and SEQ ID NO:4 except that the isoleucine at position 170 is replaced with a cysteine.
- 22. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model has a three-dimensional structure comprising atomic coordinates that have a root mean square deviation of protein backbone atoms of less than 10 angstroms when superimposed on said three-dimensional model substantially represented by the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7, and Table 8.

- 23. The invention of Claim 1, wherein said modification has an amino acid sequence that shares at least about 30% amino acid sequence homology with a FceRIa protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4.
- 24. The invention of Claim 1 or 3, wherein said model represents a FcεRIα protein having increased stability compared to the stability of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4.
- 25. The invention of Claim 1 or 3, wherein said model represents a FcεRIα protein having increased affinity for IgE compared to the affinity of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4 for IgE.
- 26. The invention of Claim 1 or 3, wherein said model represents a FcεRiα protein having altered substrate affinity compared to the affinity of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4 for IgE.
- 27. The invention of Claim 1 or 3, wherein said model comprises a three-dimensional model of a FcεRIα protein having increased solubility compared to the solubility of a human FcεRIα protein having an amino acid sequence selected from the group consisting of SEQ ID NO:2 and SEQ ID NO:4.
- 28. The invention of Claim 1, 2 or 3, wherein said model is used to identify an inhibitor of the selective binding between a FcεRIα protein and an IgE antibody.
- 29. The invention of Claim 1, 2, 3, 7, 8 or 10, wherein said model identifies crystal contacts between a FcεRIα protein and a Fc domain of an IgE antibody.
- 30. The invention of Claim 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 or 11, wherein domain 1 and domain 2 are oriented in a manner as specified by the structural coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8.
- 31. The invention of Claim 1, 2, 3, 7, 8, or 10, wherein said model identifies amino acids in the D1D2 interface.

- 32. The invention of Claim 3, wherein said method of homology modeling comprises incorporating at least a portion of the amino acid sequence of said other antibody receptor protein into said three-dimensional model substantially representing the atomic coordinates specified in a table selected from the group consisting of Table 1, Table 5, Table 6, Table 7 and Table 8 to produce said model of said other antibody receptor protein.
- 33. The invention of Claim 1, 2, 3, 4, 5, or 6, wherein said protein has an amino acid sequence selected from the group consisting of SEQ ID NO:2, SEQ ID NO:4, and SEQ ID NO:4 except that the isoleucine at position 170 is replaced with a cysteine.
- 34. The invention of Claim 4 or 5, wherein said crystal belongs to a space group selected from the group consisting of monoclinic space group C2, hexagonal space group P6₁22, and tetragonal space group P4₁.
- 35. The invention of Claim 4 or 5, wherein said crystal is selected from the group consisting of: a monoclinic space group C2 having cell dimensions of 88.6 angstroms x 69.6 angstroms x 49.3 angstroms, alpha=gamma=90.0 degrees, beta=116.69 degrees; a monoclinic space group C2 having cell dimensions of 136.02 angstroms x 75.01 angstroms x 79.28 angstroms, alpha=gamma=90 degrees, beta=117.8 degrees; a monoclinic space group C2 having cell dimensions of 136.90 angstroms x 73.79 angstroms x 79.40 angstroms, alpha=gamma=90 degrees, beta=117.74 degrees; a tetragonal space group P43 having cell dimensions of 145.08 angstroms x 145.08 angstroms x 62.74 angstroms, alpha=beta=gamma=90 degrees; a tetragonal pace group P43 having cell dimensions of 150.50 angstroms x 150.50 angstroms x 74.18 angstroms, alpha=beta=gamma=90 degrees; a hexagonal space group P6122 having cell dimensions of 58 angstroms x 58 angstroms x 226 angstroms, alpha=beta=90 degrees, gamma=120 degrees; and a hexagonal space group P6122 having cell dimensions of 58.62 angstroms x 58.62 angstroms x 229.19 angstroms, alpha=beta=90 degrees, gamma=120 degrees.
- 36. The invention of Claim 4, 5, 6, or 11, wherein said protein is produced in insect cells or Chinese hamster ovary cells.

- 37. The invention of Claim 4 or 5, wherein said crystal diffracts X-rays to a resolution selected from the group consisting of about 2.4 angstroms, about 3.1 angstroms, about 3.2 angstroms, and about 3.8 angstroms.
- 38. The invention of Claim 1, 3, 4, 5, 6, 7, 9 or 11, wherein said protein represented by said modification of Claim 1, said antibody receptor protein of Claim 3, or said FcεRIα protein of Claim 4, 5, 6, 7, 9 or 11 is selected from the group consisting of a human FcεRIα protein, a feline FcεRIα protein, a canine FcεRIα protein, an equine FcεRIα protein, a murine FcεRIα protein, and a rat FcεRIα protein.
- 39. A nucleic acid molecule comprising a nucleic acid sequence that encodes a protein selected from the group consisting of said protein of Claim 6 or 11 and said mutein of Claim 8, 9, or 10.
 - 40. A recombinant molecule comprising a nucleic acid sequence of Claim 39.
 - 41. A recombinant virus comprising a nucleic acid sequence of Claim 39.
 - 42. A recombinant cell comprising a nucleic acid sequence of Claim 39.
- 43. A method to produce a protein comprising culturing a recombinant cell of Claim 42.
- 44. An inhibitory compound identified in accordance with the method of Claim 7.
- 45. A therapeutic composition comprising an inhibitory compound of Claim 44.
- 46. A method to protect an animal from allergy, said method comprising administering to said animal an inhibitory compound of Claim 44.
- 47. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with a region of said model selected from the group consisting of the IgE binding domain, the D1D2 interface, and the clett between domain 1 and domain 2.
- 48. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with a region of said model selected from the group consisting of a A'B loop of domain 1, a EF loop of domain 1, a BC loop of domain 2, a C strand of domain 2, a CC' loop of domain 2, a C'E loop of domain 2, a F strand of domain 2, a FG loop of domain 2, and a tryptophan-containing hydrophobic ridge.

- 49. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with a region of said model in which N-linked glycosylation sites are absent.
- 50. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with an amino acid selected from the group consisting of: (a) a residue having a position in SEQ ID NO:2 or SEQ ID NO:4 selected from the group consisting of position 87, 115, 117, 118, 120-123, 128, 129, 131, 149, 153, 155 and 159; and (b) a surface residue within about 10 angstroms of any of said residues of (a).
- 51. The invention of Claim 7, 44, 45, or 46, wherein said compound interacts with an amino acid selected from the group consisting of: (a) a residue having a position in SEQ ID NO:2 or SEQ ID NO:4 selected from the group consisting of position 87, 117, 121, 123, 128, and 159; and (b) a surface residue within about 10 angstroms of any of said residues of (a).
 - 52. The invention of Claim 7, wherein said method comprises:
 - (a) generating said model, or a model of an IgE binding domain thereof, on a computer screen;
 - (b) generating the spacial structure of a compound to be tested; and
 - (c) testing to determine if said compound interacts with said IgE binding domain, wherein such an interaction indicates that said compound is capable of inhibiting said binding of an IgE antibody to a FceRIa protein.
- 53. The invention of Claim 52, wherein said step (a) includes the step of identifying one or more amino acid(s) in the IgE binding domain of said model that interact directly with the Fc domain of an IgE antibody when said Fc domain binds to said IgE binding domain.
- 54. The invention of Claim 53, wherein said compound interacts directly with one or more of said amino acid(s).
 - 55. A diagnostic reagent comprising a mutein of Claim 8, 9 or 10.
 - 56. A therapeutic composition comprising a mutein of Claim 8, 9 or 10.
- 57. A method to use a mutein of Claim 8, 9 or 10, wherein said method is selected from the group consisting of: (a) a method to protect an animal from allergy, said method comprising administering a therapeutic composition comprising said mutein

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to said animal; (b) a method to detect allergy, or susceptibility thereto, in an animal, said method comprising using said mutein to detect said allergy; and (c) a method to enhance the performance of an IgE binding assay, said method comprising incorporating into said assay said mutein.

- 58. The invention of Claim 8 or 10, wherein said step of replacing does not substantially disrupt the three-dimensional structure of said protein.
- 59. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has an increased stability compared to an unmodified antibody receptor protein.
- 60. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has an increased shelf-life compared to an unmodified antibody receptor protein.
- 61. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has a K_A for said Fc domain of at least about 3 x 10⁹ liters/mole.
- 62. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has a k_a for said Fc domain of at least about 1 x 10⁵ liters/mole-second.
- 63. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein has a k_d for said Fc domain of less than or equal to 3 x 10⁻⁵/second.
- 64. The invention of Claim 8, 9 or 10, wherein said antibody is an IgE antibody.
- 65. The invention of Claim 8, 55, 56 or 57, wherein said mutein is produced by a method comprising:
 - (a) comparing the IgE binding domain on said model with amino acid sequence of an antibody receptor protein with an improved function to identify at least one amino acid segment of said antibody receptor protein with said improved function that if incorporated into said FceRIa protein represented by said model would give said FceRIa protein said improved function; and
 - (b) incorporating said segment into said FcεRIα protein, thereby producing a mutein with said improved function.
- 66. The invention of Claim 8, 10, 55, 56 or 57, wherein said mutein is produced by a method comprising:

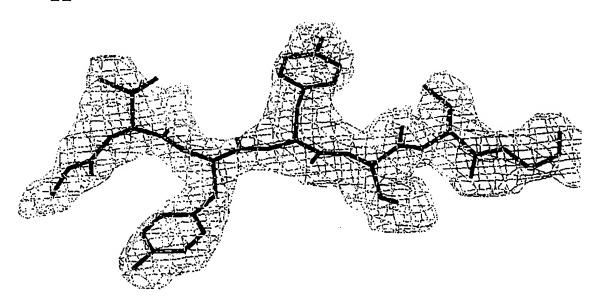
- (a) using said model to identify a three-dimensional arrangement of residues that can be randomized by mutagenesis to allow the construction of a library of molecules from which an improved function can be selected; and
- (b) identifying at least one member of said mutagenized library having said improved function.
- 67. The invention of Claim 8, 9, 10, 55, 56 or 57, wherein said mutein is produced by a method comprising:
 - (a) effecting random mutagenesis of nucleic acid molecules encoding a target of a FceRIa protein as identified by analyzing a model of that protein;
 - (b) cloning said mutagenized nucleic acid molecules into a phage display library, wherein said phage display library expresses said target; and
 - (c) identifying at least one member of the library that expresses said target, said target having an improved function.
- 68. The invention of Claim 67, wherein said target comprises an IgE binding domain and wherein said improved function comprises increased affinity of said domain for an antibody.
- 69. The invention of Claim 8 or 10, wherein said step of replacing is selected from the group consisting of:
 - (a) replacing at least one amino acid in at least one non-constrained loop of domain 1 in an area proximal to the FceRI gamma chain putative binding site;
 - (b) joining an amino-terminal amino acid residue to a carboxylterminal amino acid residue of an extracellular domain of a FcεRIα protein;
 - (c) replacing at least one amino acid site with an amino acid suitable for derivatization;
 - (d) replacing at least one pair of amino acids of said protein with a cysteine pair to enable the formation of a disulfide bond that stabilizes said mutein;
 - (e) removing at least a portion of the region between the B strand and C strand of domain 1;

- (f) removing at least a portion of the region between the C strand and E strand of domain 1;
- (g) replacing at least one amino acid in the IgE binding domain in order to increase the affinity between an IgE antibody and said protein;
- (h) replacing at least one amino acid of said protein with an amino acid such that said replacement decreases the entropy of unfolding of said protein;
- (i) replacing at least one amino acid of said protein selected from the group consisting of asparagines and glutami s with an amino acid that is less susceptible to deamidation than is said amino acid to be replaced;
- (j) replacing at least one aminc acid of said protein selected from the group consisting of methionines, histidines and tryptophans with an amino acid that is less susceptible to an oxidation or reduction reaction than is said amino acid to be replaced;
- (k) replacing at least one arginine of said protein with an amino acid that is less susceptible to dicarbonyl compound modification than is said amino acid to be replaced;
- (l) replacing at least one amino acid of said protein susceptible to reaction with a reducing sugar sufficient to reduce said protein function with an amino acid less susceptible to said reaction;
- (m) replacing at least one amino acid of said protein with an amino acid capable of increasing the stability of the inner core of said protein;
- (n) replacing at least one amino acid of said protein with at least one N-linked glycosylation site;
- (o) replacing at least one N-linked glycosylation site of said protein with at least one amino acid that does not comprise an N-linked glycosylation site; and
- (p) replacing at least one amino acid of said protein with an amino acid that reduces aggregation of said protein.

70. The invention of Claim 8, 9, 10, 55, 56 or 57, further comprising a substance attached to an amino acid of said mutein such that said substance does not substantially interfere with the antibody binding activity of said protein.

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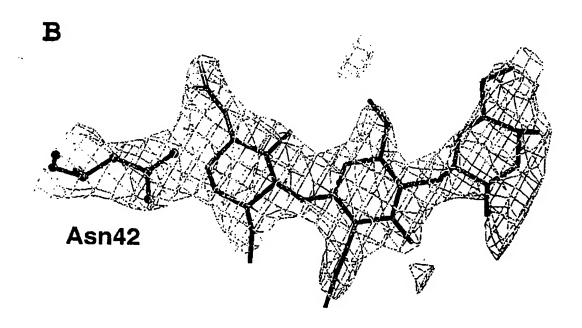
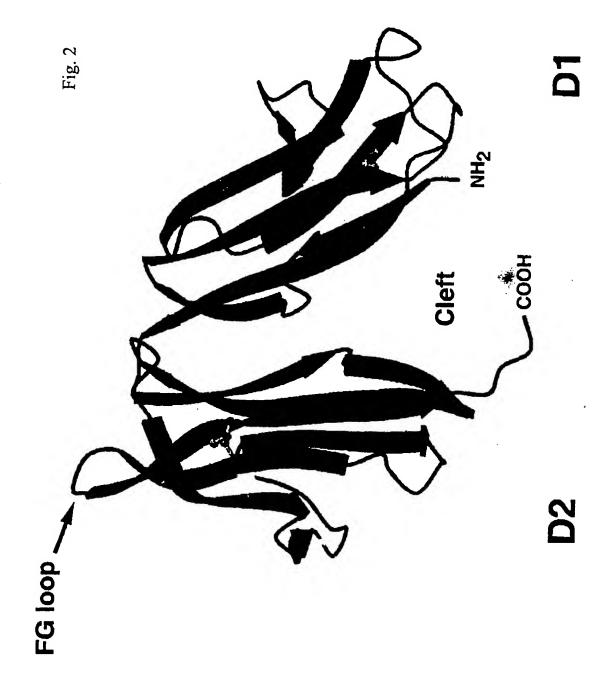
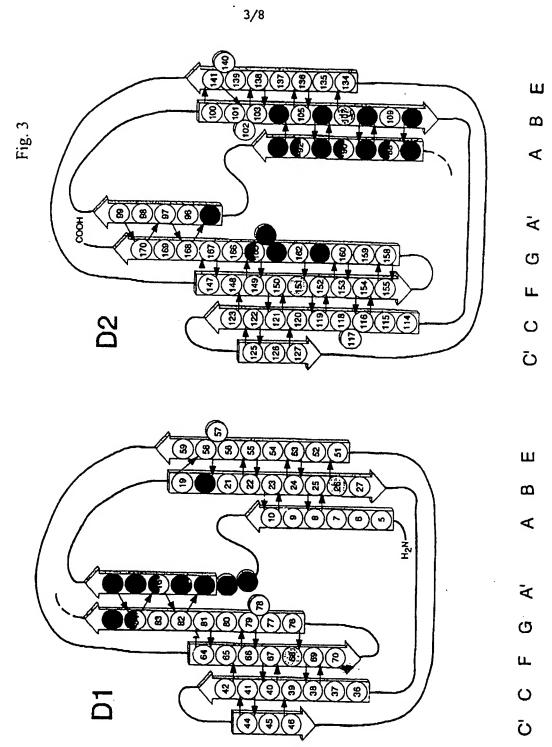
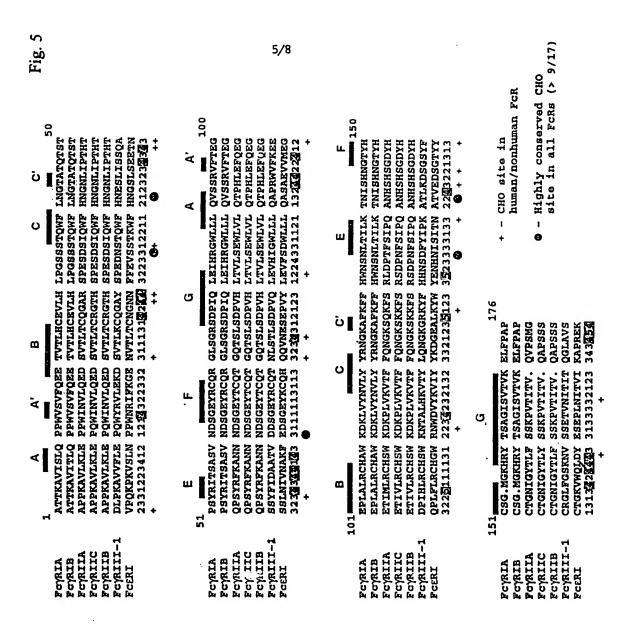


Fig. 1A, 1B

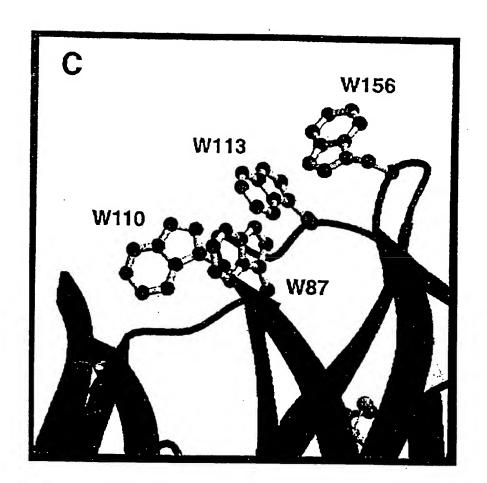






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Fig. 6



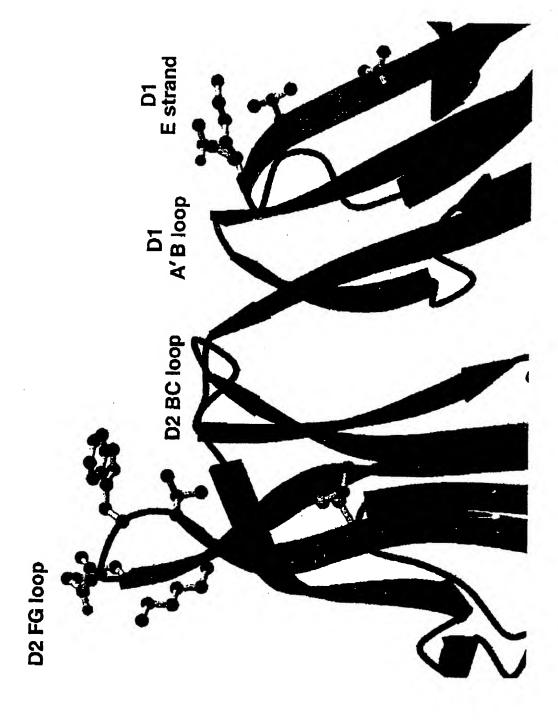
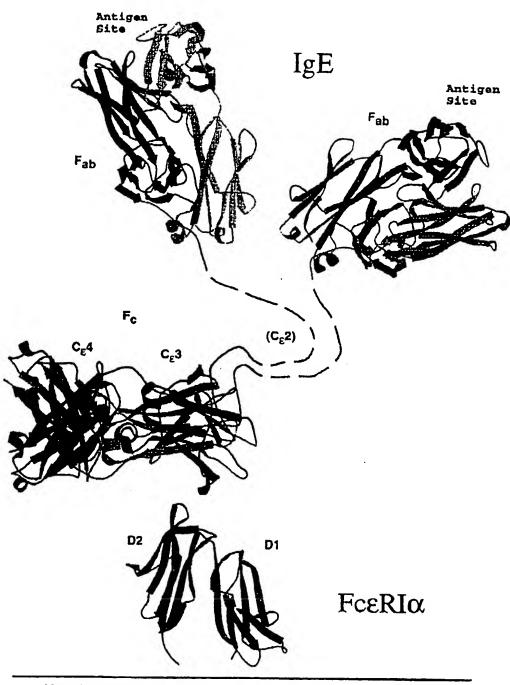


Fig. 7

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Fig. 8



Mast Cell Membrane

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Glu Val Ser Ser Thr Lys Trp Phe His Asn Gly Ser Leu Ser Glu Glu
Thr Asn Ser Ser Leu Asn Ile Val Asn Ala Lys Phe Glu Asp Ser Gly
Glu Tyr Lys Cys Gln His Gln Gln Val Asn Glu Ser Glu Pro Val Tyr
 65
                     70
Leu Glu Val Phe Ser Asp Trp Leu Leu Gln Ala Ser Ala Glu Val
                                     90
Val Met Glu Gly Gln Pro Leu Phe Leu Arg Cys His Gly Trp Arg Asn
                                105
Trp Asp Val Tyr Lys Val Ile Tyr Tyr Lys Asp Gly Glu Ala Leu Lys
Tyr Trp Tyr Glu Asn His Asn Ile Ser Ile Thr Asn Ala Thr Val Glu
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